ISOTHERM MIGRATION METHOD
IN
PHASE CHANGE PROBLEMS

A Thesis Submitted
In Partial Fulfilment of the Requirements
for the Degree of

MASTER OF TECHNOLOGY

By

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to the

DEPARTMENT OF CHEMICAL ENGINEERING

INDIAN INSTITUTE OF TECHNOLOGY KANPUR

DECEMBER, 1979

CHE-1978-M-POD-ISO

CERTIFICATE

It is certified that this work on "ISOTHERM MIGRATION METHOD IN PHASE CHANGE PROBLEMS" has been carried out under my supervision and the same has not been submitted elsewhere for a degree.

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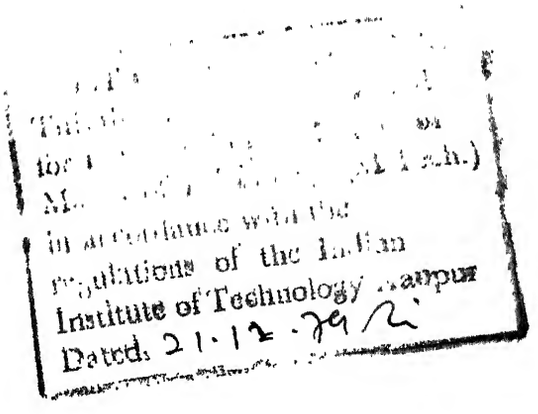

ACKNOWLEDGEMENTS

I wish to express my deep sense of gratitude to Dr. Jai P. Gupta for suggesting this interesting problem. Whatever progress I have made would have been impossible had I not the enlightening guidance, close supervision and constant encouragement from Dr. Gupta at all stages of this work.

I am very thankful to Dr. Kadalbajoo of Mathematics Department, I.I.T. Kanpur for his generous advices and fruitful suggestions in numerical computation, particularly in the stability criterion of the non-linear Partial Differential Equations.

I also thank Mr. M.K. Patra, a Senior Ph.D. student of Aeronautical Engineering Department, IIT-Kanpur who rendered a great deal of kind cooperation and help at different stages of the computer work.

I am indebted to host of my friends and colleagues for their constant encouragement and cooperation. Specifically I should name Mr. A.K. Roy who took so much of pains in polishing and proof reading the manuscripts. Successful completion of this project is due to incessant assistance and valuable informations offered by one of my close friends, Mr. S. Srinivasan.

At last but not least, I should extend my thanks to Mr. B.S. Pandey for typing this thesis, and to Mr. D.S.Panesar in preparing the drawings.

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ABSTRACT

The 'Isotherm Migration Method' has been found to be an effective numerical technique for the solution of the heat conduction problems with phase change involving temperature dependent properties. The principal equation for this method is derived with the isotherm position, $x(\theta,t)$ in the conventio heat conduction equation. This interchange of variables minimizes the computer time quite a bit compared to the other numerical methods. This is because the properties are evaluat only once at each isotherm temperature and are used throughout the computation with no need to recalculate them. In the present study, the divided difference form of the governing equation has been modified to incorporate the unequal temperat intervals in 'time-temperature' grids so that the exact proper ties obtained experimentally at unequal temperature intervals can be used in the computation without interpolation. Moreove usually the phase change temperature does not fall on one of the regular isotherms taken for convenience at round temperatu of 10°, 20°, 30° etc. or 100°, 200°, 300° etc. Hence this modified IMM enables one to use any random temperature values.

In the present work, the modified IMM has been described to determine the temperature profiles and the interface location in terms of $X(i,j)$ for unidimensional solidification of the saturated and unsaturated liquid under various geometri and different boundary conditions involving temperature

dependent properties too. The inside and outside freezing for cylindrical/spherical geometries have also been calculated by this method. The system chosen to study the method is pure water at $0^{\circ}C$ (for the saturated case) and at $20^{\circ}C$ (for the unsaturated case). The validity of the technique has been checked with good accuracy in certain cases available in the literature.

NOMENCLATURE

Symbols	Definitions
C	Specific heat of ice/water
C_1, C_2, C_3	Defined in Eqns.(29),(30) and (31), respectively
h	heat transfer coefficient of the surroundings
i	temp. indexing variable
j	time indexing variable
K	thermal conductivity of ice/water
L	suitably chosen one parameter in dimension of length
n	shape factor defined in the Eq.(1)
p	a factor to represent inward or outward solidification defined in Eqs.(39) and (43)
q_c	constant heat flux drawn from the surface
R	radius of the cylindrical/spherical geometry
R_f	interface position for the cylindrical/spherical geometry
Ri	inside radius of ithe cylindrical/spherical geometry
Ra	outside radius of the cylindrical/spherical geometry
r	position of the isotherm at any time in the cylindrical/spherical body
T	dimensionless temperature defined by $= \frac{\theta - \theta_w}{\theta_o - \theta_w}$ for B.C. of the 1st kind in the solid zone $= \frac{\theta \cdot K_o}{q_c \cdot L}$ for B.C. of the 2nd kind in planer geometry $= \frac{\theta \cdot K_o}{q_c \cdot R}$ for B.C. of the 2nd kind in cylindrical/spherical geometry

$= \frac{\theta - \theta_\infty}{\theta_o - \theta_\infty}$ for B.C. of the 3rd kind in the solid zone

$= \frac{\theta_s - \theta}{\theta_s - \theta_o}$ for B.C.s of the 1st and 3rd kind in the liquid zone

T(i) Dimensionless temperature of the ith isotherm

TKI Defined in Eq.(32)

t time

X dimensionless position of the isotherm

X(i,j) the position of the ith isotherm at jth time

XI defined in Eq.(33)

XA defined in Eq.(27)

XB defined in Eq.(28)

x distance from the surface

$\dot{x}$ speed of the isotherm

α thermal diffusivity of ice/water

θ temperature

λ latent heat of solidification of water at the interface temperature

ρ density of ice/water

τ dimensionless time

$= \alpha_o \, t/L^2$ for planar system

$= \alpha_o \, t/R^2$ for cylindrical/spherical system

Subscripts

0 evaluated at the interface position in the solid state

s initial state for the unsaturated liquid

w evaluated at the surface of the geometries

1 for solid state

2 for liquid state

∞ evaluated at bulk of the surroundings

CHAPTER 1

INTRODUCTION

1.1 The Importance of Solidification/Melting Problems:

The change of state occurring with melting or freezing is associated with many of today's industrially relevant problems. The heat transfer problem with phase change is evident in the solidification of casting, freezing, thawing of soils and foodstuffs, preservation of medical and biochemical materials, thermal storage devices, the ablation of missile skins under aerodynamics, heating, welding etc. Because of the economic importance of such processes, a wide range of research in the effects of phase change and in the physical models for it has been conducted.

1.2 Difficulties in Establishing an Exact Solution for the Solidification/Melting Problems:

In the transient heat conduction problem, the supply or removal of heat from any element causes it to change its temperature. In the case of solidification or melting, however, the system is essentially complicated due to the release or absorption of the latent heat of fusion which brings the non-linearity in the governing differential equations.

1.3 Different Approaches to Solve the Phase Change Problems:

A variety of approaches to the solution of phase change problems in solidification or melting classified as 'Stefan's Problems' have been used by different investigators. Solutions have been obtained for various geometries and boundary conditions for well over hundred years. After the reviews by Bankoff [12] and Muehlbauer et al.[13], over 400 papers have appeared in the International Journals [14]. Since exact analysis is difficult for all but very simple problems, various approximations have been used by different investigators. These namely are conformal mapping, embedding technique, finite element method, heat balance integral technique, integral equation method, iterative analytical method, numerical methods, perturbation method etc. Most of the above methods assume constant thermophysical properties for the system which is far from the reality. In some cases linear or other kinds of variations in properties with temperature are assumed. These are generally solved by the conventional numerical method, where space and time grids are used. The properties are evaluated at each grid point due to the change in temperature at the grids with the passage of time. This results in excess computer time usage.

1.4 A New Numerical Approach 'Isotherm Migration Method'(IMM):

An effective way out has been suggested [1,2] to transform the conventional heat conduction equation so that

its solutions express space as a function of the temperature and time coordinates. Instead of writing temperature $\theta = \theta(x,t)$, one expresses 'x' as a function of temperature and time i.e. $x=x(\theta,t)$. Then, using conventional numerical technique the positions of the various isotherms at different times are calculated. Hence one essentially traces the movement of the isotherms (i.e. constant temperature lines) at different times. So it is called the ISOTHERM MIGRATION METHOD (IMM). This obviates the need to calculate the properties at each grid point. The values of the properties once calculated, can be used throughout the computation with no need to recalculate them. This process minimizes the computer time quite a bit. The efficacy of this technique over other approximate methods lies in the heat transfer and diffusion problems with property variation. Apart from this, in ablation analysis the effect of surface recession is more easily treated. The temperature distribution is more readily applicable to thermal stress analysis since more points occur in the region of large temperature gradients usually at the specimen surfaces.

1.5 Literature Review on IMM:

Chernousko [1] has explored this idea for the solution of non-linear heat conduction problems in a medium with phase change. Dix and Cizek [2] used this technique

for transient heat conduction analysis in one dimension for the boundary condition of the third kind. Crank and Phahle [3] have applied this method to solve the problem of the melting of a plane sheet of ice. Crank and Gupta [5] have extended the IMM to two dimension system evaluating the problem posed by the solidification of a square prism of fluid initially at constant temperature.

1.6 The Modification of the Existing IMM in the Present Study and the Advantage Therein:

In the present study the IMM has been modified to include unequal temperature grids in the finite difference form for the numerical calculations. This modification eliminates certain shortcomings in the existing IMM. The existing formulation of the IMM requires the use of constant temperature intervals which often lead to interpolation between values of properties obtained experimentally at specific temperatures. More serious is the fact that the phase change temperature does not usually fall on one of the regular isotherms taken conveniently at round temperature of 10^{o}, 20^{o}, 30^{o} etc. or 100^{o}, 200^{o}, 300^{o} etc. Hence, this modification helps to use the exact properties at unequal temperature intervals reported in the literature, without interpolation. This also cuts down the computer time a bit and gives less erroneous results. This method can conveniently be extended to solve multiphase solidification problems where interface

temperatures usually are not at regular intervals.

1.7 Focus on the Details of the Present Work:

It is known that a solution to a problem in solidification is also a solution to the corresponding inverse problems in melting, the present work has been arbitrarily restricted to the process of solidification in order to facilitate the detailed search.

The modified IMM has been used to calculate the interface location and the temperature profiles as a function of time for a undimensional solidifying system subjected to any possible combination of the following conditions:

1. Solidification can take place in Cartesian, cylindrical or spherical geometries.
2. The boundary condition at the surface of the body can be of the 1st, 2nd or the 3rd kind.
3. In the case of cylindrical or spherical body the solidification can proceed outward or inward.
4. Initial state of the liquid could be at the freezing temperature θ_o (saturated case) or at any temperature θ_s above the fusion temperature (unsaturated case).
5. The property variation as a function of temperature in the system (both in the solid and liquid region) can also be taken into account.

6. The temperature intervals can be equally or unequally spaced in the time-temperature grid.

The system treated in each case is further defined by the following postulates: (a) The phase change occurs at a fixed temperature, the fusion temperature (θ_o). (b) Convection effects on heat transfer due to density change has been ignored. (c) Initially the liquid is at a uniform temperature. (d) In the constant property and unsaturated case, the property of solid and liquid has separately been evaluated at the fusion temperature (θ_o).

CHAPTER 2

MATHEMATICAL FORMULATIONS

2.1 The Transformed Equation for IMM and the Significance of Each Term Involved:

The heat conduction equation in one dimension system without internal heat generation is expressed as

$$\rho c \frac{\partial \theta}{\partial t} = \frac{1}{x^n} \frac{\partial}{\partial x} \left[(K x^n \frac{\partial \theta}{\partial x}) \right] \qquad (1)$$

Here n is called the shape factor.

n = 0 planar geometry

n = 1 cylindrical geometry

n = 2 spherical geometry

Eq.(1) can be transformed to the desired form to suit IMM with the help of following relations:

$$(\frac{\partial \theta}{\partial x}) = (\frac{\partial x}{\partial \theta})^{-1} \qquad (2)$$

and

$$(\frac{\partial \theta}{\partial t})_x = - (\frac{\partial \theta}{\partial x})_t (\frac{\partial x}{\partial t})_\theta \qquad (3)$$

Substituting Eqs (2) and (3) in Eq.(1), we have

$$\rho c \left\{ -(\frac{\partial \theta}{\partial x})(\frac{\partial x}{\partial t}) \right\} = \frac{1}{x^n} \left\{ \frac{\partial}{\partial \theta} [K x^n (\frac{\partial x}{\partial \theta})^{-1}] \frac{\partial \theta}{\partial x} \right\}$$

$$= \frac{1}{x^n} \left\{ \frac{\partial}{\partial \theta} (K x^n) (\frac{\partial x}{\partial \theta})^{-1} + (K x^n) \cdot \frac{\partial}{\partial \theta} (\frac{\partial x}{\partial \theta})^{-1} \right\} \left(\frac{\partial x}{\partial \theta} \right)^{-1}$$

$$= \frac{1}{x^n}\left\{\frac{\partial}{\partial\theta}(K\,x^n)\,(\frac{\partial x}{\partial\theta})^{-2} - (K\,x^n)(\frac{\partial x}{\partial\theta})^{-3}(\frac{\partial^2 x}{\partial\theta^2})\right\}$$

$$= \frac{1}{x^n}\left\{(\frac{\partial K}{\partial\theta}\,x^n + K.n.x^{n-1}\,(\frac{\partial x}{\partial\theta}))\cdot(\frac{\partial x}{\partial\theta})^{-2}\right.$$

$$\left. - K\,x^n\,(\frac{\partial x}{\partial\theta})^{-3}(\frac{\partial^2 x}{\partial\theta^2})\right\}$$

Cancelling $(\frac{\partial x}{\partial\theta})^{-1}$ from both sides of the equation, we have

$$-\rho C\,(\frac{\partial x}{\partial t}) = \left\{((\frac{\partial K}{\partial\theta}) + \frac{K\,n}{x}\,(\frac{\partial x}{\partial\theta})(\frac{\partial x}{\partial\theta})^{-1} - K(\frac{\partial x}{\partial\theta})^{-2}(\frac{\partial^2 x}{\partial\theta^2})\right\}$$

or

$$(\frac{\partial x}{\partial t}) = \frac{K}{\rho C}\left\{(\frac{\partial^2 x}{\partial\theta^2})(\frac{\partial x}{\partial\theta})^{-2} - \frac{n}{x} - \frac{1}{K}\,(\frac{\partial K}{\partial\theta})(\frac{\partial x}{\partial\theta})^{-1}\right\}$$

or

$$(\frac{\partial x}{\partial t}) = \dot{x} = \alpha\left\{(\frac{\partial^2 x}{\partial\theta^2})(\frac{\partial x}{\partial\theta})^{-2} - \frac{n}{x} - \frac{1}{K}\,(\frac{\partial K}{\partial\theta})(\frac{\partial x}{\partial\theta})^{-1}\right\} \qquad (4)$$

Thus Eq.(4) becomes the governing equation expressed in terms of $x(\theta, t)$ for the one dimensional unsteady state heat conduction. The left hand side of eq.(4), indeed represents the migration rate of a particular isotherm (θ) as a function of time. The first term on the right hand side of Eq.(4) implies the migration rate of the isotherm through the geometry whose surface area is not a function of thickness (i.e. planar system) and the thermophysical properties are independent of temperature. The second term takes into consideration of the shape factor to include the cylindrical and the spherical geometries. The last term accounts for

the temperature dependence of α and K. The above Eq.(4) has already been derived from energy balance [2] which provides better insight into the physical situation and allows easier incorporation of the other effects, for example, phase change and temperature dependent heat generation.

2.2 Different Boundary Conditions Studied for the Solidification Problem:

The IMM has been used for a unidimensional solidifying system whose surface is exposed to the following boundary conditions.

(a) The boundary condition of the 1st kind is

$$\theta = \theta_w \quad \text{at } x=0, \quad t \geq 0 \tag{5}$$

(b) The boundary condition of the 2nd kind is

$$q_c = K \frac{\partial \theta}{\partial x} = K\left(\frac{\partial x}{\partial \theta}\right)^{-1} \quad \text{at } x=0, \quad t \geq 0 \tag{6}$$

(c) The boundary condition of the 3rd kind is

$$K \frac{\partial \theta}{\partial x} = h(\theta_w - \theta_\infty) \quad \text{at } x=0, \quad t \geq 0$$

$$K \left(\frac{\partial x}{\partial \theta}\right)^{-1} = h\,(\theta_w - \theta_\infty) \tag{7}$$

The condition at the solid-liquid interface describing the process of solidification is

$$K_1\left(\frac{\partial x}{\partial \theta}\right)_1^{-1} - K_2\left(\frac{\partial x}{\partial \theta}\right)_2^{-1} = \rho_o \ell \left(\frac{\partial x}{\partial t}\right) \tag{8}$$

$$\text{at } x=x_o$$

The equation is valid for the solidification of the unsaturated liquid initially at the temperature (θ_s). For the saturated liquid Eq.(8) simplifies to

$$K_1\left(\frac{\partial x}{\partial \theta}\right)_1^{-1} = \rho_o \lambda \left(\frac{\partial x}{\partial t}\right) \qquad (9)$$

at $x=x_o$

The initial conditions are defined as

$$\theta = \theta_s \quad \text{for the unsaturated liquid} \qquad (10)$$

and $$\theta = \theta_o \quad \text{for the saturated liquid} \qquad (11)$$

2.3 Non-dimensionalisation of the Transformed Equation and the Boundary Conditions Involved:

To generalise the application of the IMM so that any phase change problem can easily be treated with the one governing equation, it is required to non-dimensionalise Eq.(4) and also the boundary conditions involved. The choice of variables to define the dimensionless parameter is made according to the boundary conditions and shapes describing the solidification system.

(a) Boundary Condition of the 1st kind.

$$T_1 = \frac{\theta - \theta_w}{\theta_o - \theta_w}, \qquad T_2 = \frac{\theta_s - \theta}{\theta_s - \theta_o}$$

$$\tau = \alpha_o\, t/L^2, \quad \text{for plane system}$$

$$= \alpha_o\, t/R^2, \quad \text{for cylindrical/spherical system}$$

and $X = x/L$ for planar system

$= r/R$ for cylindrical/spherical system

Substituting the above dimensionless parameter, the Eq.(4) takes the form

$$\frac{\partial X}{\partial \tau} = \frac{\alpha}{\alpha_o}\left[\left(\frac{\partial^2 X}{\partial T^2}\right)\left(\frac{\partial X}{\partial T}\right)^{-2} - \frac{n}{X} - \frac{1}{K}\left(\frac{\partial K}{\partial T}\right)\left(\frac{\partial X}{\partial T}\right)^{-1}\right] \tag{12}$$

The dimensionless Eq.(12) gives the location of different isotherms both in the solid and the liquid region as denoted by the subscripts 1 and 2 respectively.

The Eq.(8), representing the interface location, takes the form

$$\left[K_1\left(\frac{\partial X}{\partial T}\right)_1^{-1}(\theta_o - \theta_w) + K_2\left(\frac{\partial X}{\partial T}\right)_2^{-1}(\theta_s - \theta_o)\right]\cdot L = \rho_o \lambda \left(\frac{\partial X}{\partial \tau}\right)\cdot L\cdot \alpha_o$$

$$\text{Or,}\quad \left[K_1\left(\frac{\partial X}{\partial T}\right)_1\cdot(\theta_o - \theta_w) + K_2\left(\frac{\partial X}{\partial T}\right)_2^{-1}(\theta_s - \theta_o)\right] = \rho_o \lambda \alpha_o \left(\frac{\partial X}{\partial \tau}\right)$$

$$\text{at } X = X_o \tag{13}$$

The Eq.(13) is applicable for the unsaturated liquid, while for the saturated liquid the Eq.(9) takes the form

$$K_1\left(\frac{\partial X}{\partial T}\right)_1^{-1}(\theta_o - \theta_w) = \rho_o \lambda \alpha_o \left(\frac{\partial X}{\partial \tau}\right)$$

$$\text{Or,}\quad \left(\frac{\partial X}{\partial \tau}\right) = \frac{C_o(\theta_o - \theta_w)}{\lambda}\left(\frac{\partial X}{\partial T}\right)_1^{-1} \tag{14}$$

The boundary condition at X=0 and $\tau \geq 0$

$$T = 0 \tag{15}$$

(b) The boundary condition of the 2nd kind.

Here the dimensionless parameters are

$$T = \frac{K_o \cdot \theta}{q_c \cdot L} \quad \text{for planar system}$$

$$= \frac{K_o \cdot \theta}{q_c \, R} \quad \text{for cylindrical/spherical system}$$

and

$$\tau = \alpha_o \, t/L^2 \text{ for planar system}$$

$$= \alpha_o \, t/R^2 \text{ for cylindrical/spherical system}$$

and $X = x/L$ for planar system

$= r/R$ for cylindrical/spherical system

With these parameters Eq.(4) transforms again into Eq.(12), whereas Eqs (8) and (9) become

$$\frac{\partial X}{\partial \tau} = \frac{q_c \cdot L}{\rho_o \lambda \alpha_o} \left[\frac{K_1}{K_o} \left(\frac{\partial X}{\partial T}\right)_1^{-1} + \frac{K_2}{K_o} \left(\frac{\partial X}{\partial T}\right)_2^{-1} \right]$$

$$\text{or,} \quad \left(\frac{\partial X}{\partial \tau}\right) = \frac{q_o \cdot L}{\rho_o \lambda \alpha_o} \left[\left(\frac{\partial X}{\partial T}\right)_1^{-1} + \frac{K_2}{K_o} \left(\frac{\partial X}{\partial T}\right)_2^{-1} \right] \qquad (16)$$

[At the interface $K_1 = K_o$]

$$\text{and} \quad \left(\frac{\partial X}{\partial \tau}\right) = \frac{q_c \cdot L}{\rho_o \lambda \alpha_o} \left(\frac{\partial X}{\partial T}\right)_1^{-1} \qquad (17)$$

$$\text{at } X = X_o$$

for unsaturated and saturated liquid respectively. The boundary condition at X=0, and $\tau \geq 0$, i.e. at the surface represented by the Eq.(6), becomes

$$\frac{K}{K_o}\left(\frac{\partial X}{\partial T}\right)^{-1} = 1 \qquad (18)$$

(c) The boundary condition of the 3rd kind.

Here the dimensionless parameters chosen are:

$$T_1 = \frac{\theta - \theta_\infty}{\theta_o - \theta_\infty}, \qquad T_2 = \frac{\theta_s - \theta}{\theta_s - \theta_o}$$

$\tau = \alpha_o\, t/L^2$ for planar system

$= \alpha_o\, t/R^2$ for cylindrical/spherical system

$X = x/L$ for planar system

$= r/R$ for cylindrical/spherical system

Here also Eq.(4) transforms into eq.(12), whereas Eqs.(8) and (9) become

$$\left[K_1\left(\frac{\partial X}{\partial T}\right)_1^{-1}(\theta_o - \theta_\infty) + K_2\left(\frac{\partial X}{\partial T}\right)_2(\theta_s - \theta_o)\right] = \rho_o \lambda \alpha_o \left(\frac{\partial X}{\partial \tau}\right) \qquad (19)$$

and

$$\left(\frac{\partial X}{\partial \tau}\right) = \frac{(\theta_o - \theta_\infty)\, C_o}{\lambda}\left(\frac{\partial X}{\partial T}\right)_1^{-1} \qquad (20)$$

at $X = X_o$ respectively.

The boundary condition at X=0 and $\tau \geq 0$, i.e. at the surface represented by Eq.(7), takes the form.

$$\left(\frac{\partial T}{\partial X}\right) = \frac{h.L.}{K} \cdot T_w \qquad (21)$$

The initial conditions which are same for all the B.C.s are

$T_2 = 1$ for unsaturated liquid; $T_1 = 1$ for saturated liquid (22)

The numerical solution of Eq.(12) with different boundary conditions has been dealt with in Chapter 3.

CHAPTER 3

NUMERICAL CALCULATIONS

At first, it is observed that the transformed Eq.(4) or Eq.(12) is non-linear even for the constant thermal properties and Cartesian system, whereas the original heat conduction equation is linear. This is relatively unimportant if an explicit difference method is used as in Eq.(25), but would call for the solution of a set of non-linear algebraic equations if an implicit difference method is introduced. Hence explicit or forward difference method [10] is used here. The non-linearity causes no problem in applying this method.

3.1 Divided Difference Form for the Governing Equation and the Boundary Conditions:

To incorporate the unequal temperature interval in (τ-T) grid for the numerical solution, the finite difference form for the 2nd order derivative is expressed in the following form:

$$\frac{\partial^2 X}{\partial T^2} = \frac{\left[\frac{X(i+1,j)-X(i,j)}{T(i+1)-T(i-1)}\right] - \left[\frac{X(i,j)-X(i-1,j)}{T(i)-T(i-1)}\right]}{(T(i+1)-T(i-1))/2} \qquad (23)$$

If the temperature interval is equally spaced, i.e. $T(i+1)-T(i) = T(i)-T(i-1) = \Delta T$, then Eq.(23) simplifies to the conventional form

$$\frac{\partial^2 X}{\partial T^2} = \frac{X(i+1,j) - 2X(i,j) + X(i-1,j)}{(\Delta T)^2} \qquad (24)$$

So, forward difference in time and central difference in temperature yield an equation from the Eq.(12) for the ith isotherm position at the time (j+1) as follows:

$$\frac{X(i,j+1)-X(i,j)}{\Delta\tau} = \frac{\alpha(i)}{\alpha_o}\Big[\Big(\frac{\frac{X(i+1,j)-X(i,j)}{T(i+1)-T(i)} - \frac{X(i,j)-X(i-1,j)}{T(i)-T(i-1)}}{(T(i+1)-T(i-1))/2}\Big)$$

$$\Big(\frac{X(i+1,j)-X(i-1,j)}{T(i+1)-T(i-1)}\Big)^{-2} - \frac{n}{X(i,j)} - \frac{1}{K(i)}\Big(\frac{K(i+1)-K(i-1)}{T(i+1)-T(i-1)}\Big)\cdot$$

$$\Big(\frac{X(i+1,j)-X(i-1,j)}{T(i+1)-T(i-1)}\Big)^{-1}\Big]$$

$$= \frac{\alpha(i)}{\alpha_o}\Big[2\cdot\Big(\frac{\frac{X(i+1,j)-X(i,j)}{T(i)-T(i-1)} - \frac{X(i,j)-X(i-1,j)}{T(i)-T(i-1)}}{X(i+1,j)-X(i-1,j))^2}\Big)\cdot(T(i+1)-T(i-1))$$

$$- \frac{n}{X(i,j)} - \frac{K(i+1)-K(i-1)}{K(i)\,(X(i+1,j)-X(i-1,j))}\Big] \qquad (25)$$

The Eq.(25) can be simplified to the form

$$X(i,j+1) = (XA+XB)\cdot C_1 + (1-C_2)\cdot X(i,j) - \frac{C_3\, n}{X(i,j)} - \frac{C_3\, TKI}{K(i)\cdot XI} \qquad (26)$$

where

$$XA = X(i+1,j)\cdot(T(i)-T(i-1)) \qquad (27)$$

$$XB = X(i-1,j)\cdot(T(i+1)\cdot T(i)) \qquad (28)$$

$$C_1 = \frac{\alpha(i)}{\alpha_o}\,\Delta\tau\Big(\frac{2(T(i+1)-T(i-1))}{(X(i+1,j)-X(i-1,j))^2\cdot(T(i+1)-T(i))(T(i)-T(i-1)}\Big) \qquad (29)$$

$$C_2 = C_1\,(T(i+1)-T(i-1)) \qquad (30)$$

$$C_3 = \frac{\alpha(i)}{\alpha_o} \cdot \Delta\tau \tag{31}$$

$$TKI = K(i+1) - K(i-1) \tag{32}$$

$$XI = (X(i+1,j) - X(i-1,j)) \tag{33}$$

Similarly the finite difference form for the boundary conditions at the interface and at the wall for different cases becomes.

(a) For B.C. of the 1st kind

At $X = X_o$

$$X(i,j+1) = X(i,j) + \frac{\Delta\tau}{\alpha_o \rho_o \lambda}\cdot[K_1(\theta_o - \theta_w)\cdot\left(\frac{X(i,j)-X(i-1,j)}{T(i) - T(i-1)}\right)^{-1} + K_2(\theta_s-\theta_o)\left(\frac{X(i+1,j)-X(i,j)}{T(i+1)-T(i)}\right)^{-1}] \tag{34}$$

For saturated liquid it becomes

$$X(i,j+1) = X(i,j) + \left[\frac{\Delta\tau\cdot C_o(\theta_o - \theta_w)\cdot(T(i)-T(i-1))}{(X(i,j) - X(i-1,j))}\right] \tag{35}$$

At $X=0$, $\tau \geqslant 0$

$X(1,j) = 0$ for planer system

$X(1,j) = 1.0$ for cylindrical/spherical system

(b) For B.C. of the 2nd kind

At $X=X_o$ The Eqs(16) and (17) become

$$X(i,j+1) = X(i,j) + \left(\frac{\Delta\tau\cdot q_c\cdot L}{\alpha_o \rho_o \lambda}\right)\left[\frac{X(i,j)-X(i-1,j)}{T(i)-T(i-1)}\right)^{-1} - \frac{K_2}{K_o}\left(\frac{X(i+1,j) - X(i,j)}{T(i+1) - T(i)}\right)^{-1}] \tag{36}$$

and

$$X(i,j+1) = X(i,j) + \frac{(q_c \Delta\tau L)\cdot(T(i)-T(i-1))}{(\alpha_o \rho_o \lambda)\cdot(X(i,j)-X(i-1,j))} \qquad (37)$$

At the surface i.e. X=0 and $\tau \geq 0$, the corresponding Eq.(18) becomes

$$T_w = \left[T(2) - X(2,j+1)\right] /K(i)/K_o \qquad (38)$$

Eq.(38) is for planer system, while for cylindrical and spherical system the Eq.(18) takes the form:

$$T_w = \left[T(2) + (p\cdot(1-X(2,j+1)))\right]/K(i)/K_o \qquad (39)$$

Here p=1 for inside solidification and p=-1 for the outside solidification.

(c) For B.C. of the 3rd kind

At $X=X_o$, Eqs.(16) and (17) for the unsaturated and saturated liquid become

$$X(i,j+1) = X(i,j) + \frac{\Delta\tau}{\alpha_o \rho_o \lambda}\left[K_1(\theta_o - \theta_\infty)\left(\frac{X(i,j)-X(i-1,j)}{T(i) - T(i-1)}\right)^{-1}\right.$$

$$\left. + K_2(\theta_s - \theta_o)\left(\frac{X(i+1,j)-X(i,j)}{T(i+1)-T(i)}\right)^{-1}\right] \qquad (40)$$

and

$$X(i,j+1) = X(i,j) + \frac{\Delta\tau\, C_o(\theta_o - \theta_{co})\cdot(T(i)-T(i-1))}{\lambda\,(X(i,j) - X(i-1,j))} \qquad (41)$$

At the surface of the body i.e. X=0, $\tau \geq 0$, the finite difference form of Eq.(19) becomes,

$$T_w = T(2)/(1 + \frac{X(2,j+1)\cdot h.L}{K(1)}) \text{ for planer system} \quad (42)$$

$$= T(2)/(1+p\cdot(\frac{(1-X(2,j+1))\cdot h.L}{K(1)})) \text{ for cylindrical/spherical system} \quad (43)$$

Here also p=1 for inside freezing and p= -1 for outside freezing.

3.2 Convergence, Stability Criterion and Truncation Error:

The explicit scheme necessitates the convergence and the stability criterion to be satisfied to implement the numerical solution. The convergence implies that the finite difference approximation will approach the exact solution when the size of the increments employed is made infinitesimally small. The stability implies that errors associated with the use of increments of finite size or round off error will not grow as the calculation proceeds. When finite difference procedure is both convergent and stable, a comparison of the calculations made using two different increment intervals is generally a good indication of the reliability that may be assigned to the results. Although some definite tests are available for the convergence and stability criterion of the linear equations, but, no straight forward treatment to the convergence and the stability of the non-linear equations is readily available. In this situation, one must proceed with

the physical concept of the formulations.

The stability criterion for non-linear equations can be approximated in the following manner:

(i) The non-linear equation, if possible, is simplified to the linear form, just by eliminating some parameters or variables involved. Then the stability criterion for the simplified linear equation is found. Now small variation or perturbation is intuitively given to the determined value to take into account the non-linear effect/effects of the main equation. Finally one should accept that perturbated value of the stability criterion for which convergence criterion is achieved.

(2) If it is not possible to simplify into the linear form, then, intuitively satisfying the physical concept of the problem, one can establish a relation from the coefficients of the divided difference form of the non-linear equation.

The governing Eq.(12) belongs to the second category. Eq.(12), even for the simplest case like planer geometry and constant property, is non-linear and its divided difference form i.e. Eq.(26) simplifies to the expression

$$X(i,j+1) = (XA + XB)\cdot C_1 + (1 - C_2)X(i,j) \qquad (44)$$

Now for $X(i,j+1)$ to increase with an increase in $X(i,j)$, as expected physically the coefficient of $X(i,j)$ must be positive i.e.,

$$(1 - C_2) \geq 0$$

$$\alpha_1 \left[1 - \frac{\alpha(i)}{\alpha_o}\left(\frac{2(T(i+1)-T(i-1))^2 \Delta\tau}{(X(i+1,j)-X(i-1,j))^2 (T(i+1)-T(i))\cdot(T(i)-T(i-1))}\right)\right] > 0$$

This finally yields

$$\Delta\tau < \frac{(X(i+1,j)-X(i-1,j))^2 (T(i+1)-T(i))(T(i)-T(i-1))}{2\cdot(T(i+1) - T(i-1))\cdot(\alpha(i)/\alpha_o)} \tag{45}$$

Since the equation is non-linear a more exact analysis is not possible. For the equal temperature interval, the expression (45) simplifies to the form as given in [2]

$$\Delta\tau < (X(i+1,j) - X(i-1,j))^2/8.(\alpha(i)/\alpha_o) \tag{46}$$

or in the dimensional form

$$\Delta t < (x(i+1,j) - x(i-1,j))^2/8.\alpha\ (i) \tag{47}$$

From a comparison of the Taylor series representation of Eq.(12) and its differential equivalent, the truncation error is found to be proportional to $(\Delta\tau)$ and $(\Delta T)^2$ which compare with $(\Delta\tau)$ and $(\Delta X)^2$ for the explicit equation.

3.3 Computational Procedure for Different Cases:

It is evident from Eq.(26) and the boundary conditions at X=0 and $X=X_o$, that if X(i,j) is known at one time τ one can compute the X(i,j) at $(\tau+\Delta\tau)$ time i.e. X(i,j+1). This

corresponds to all isotherms chosen including the interface one. This implies that the present state of the system can be evaluated by this explicit technique if the past state of the system is known. Thus one must generate an initial set of isotherms to begin the IMM. Analytic or some alternative solution is needed to provide the temperature distribution at some small time from which IMM can proceed on. In the present study the analytical solutions [4,9 and 15] have been used, according to the different cases to initialise the isotherm locations including the interface isotherm for small time t=1 min. In certain cases this IMM has been used to compute the solidification even upto 10 hours. The results thus obtained are found to be in good agreement with [4]. For clarity in the graphs only the computations upto 1 hour have been plotted in all the cases.

For very short times the cylindrical and spherical solutions approach the planar solution. Accordingly, the results of the planar solution [4] for t=1 min have been used to start the IMM in the cylindrical and spherical cases. The small error from this approximation dies out rapidly with time as was confirmed by the calculation done with different initial temperature distribution.

For the boundary condition of the 2nd and 3rd kind, the rate of surface temperature increase is determined from an energy balance near the surface as represented in Eqs.(38,39,42 and 43). The first appearance of the new isotherm has been located inside the body near the wall by linear approximation with those of other existing isotherms. It does not affect the result because

the temperature intervals chosen are small enough like -5°, -4°, -3°, -2°, -1°, 0°C so on. As the surface temperature decreases, the new isotherms must be created at the boundary and allowed to migrate into the medium.

The time increment $\Delta\tau$ has been calculated satisfying the stability criterion from the Eq.(45). To calculate $\Delta\tau$ from Eq. (45), the two alternate isotherms nearer to the surface have been taken because they are closely spaced in comparison to other distant isotherms. After every five iterations $\Delta\tau$ has been recalculated from the Eq.(45) since the spatial distance between any two isotherms increases as the time progresses. This procedure also reduces the amount of computation time. The effects of 3rd and 4th terms in Eq.(26) for cylindrical/spherical geometry and property variation respectively have been taken into account, choosing conveniently $\Delta\tau = 0.75\left[\Delta\tau\right]_{\text{calculated}}$. This is so because their contribution in the main Eq.(26) is small for the system studied. It has been found that in case of inside solidification, for cylinder or sphere, the computation becomes unstable even before reaching the neighbourhood of the centre. Since X(i,j) becomes lower, the 3rd term in Eq.(26) dominates and ceases to give the right solution. To combat this situation $\Delta\tau$ has been cut short accordingly in different stages of computations so that solidification can be achieved upto the neighbourhood of the centre. The complete solidication has been calculated by extrapolating the situations of partial solidifications upto the neighbourhood of the centre.

CHAPTER 4

FLOW DIAGRAM OF THE COMPUTER PROGRAMMING

The outline of the computer programming comprising of all the system variables studied in the present work has been shown below in the form of block diagrams. The listing of the final FORTRAN IV program is given in the Appendix II.

Codes used in the program and their significances with appropriate values:

(a) Geometry types (N)

= o Planar geometry
= 1 Cylindrical geometry
= 2 Spherical geometry

(b) Boundary conditions (KOD)

= -1 Boundary condition of the 1st kind
= 0 Boundary condition of the 2nd kind
= 1 Boundary condition of the 3rd kind

(c) Initial state of the liquid (NIS)

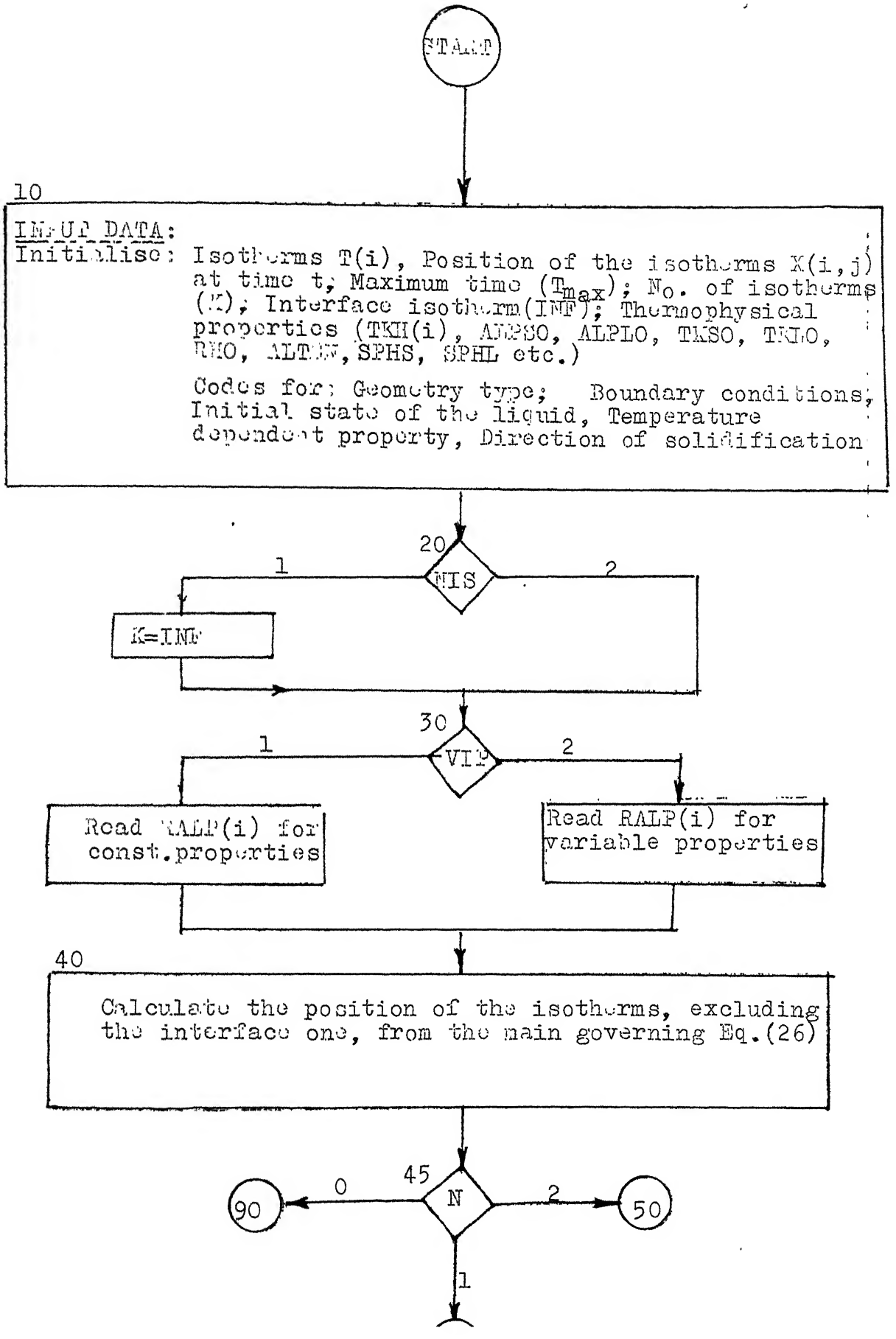
= 1 Solidification of saturated liquid
= 2 Solidification of unsaturated liquid

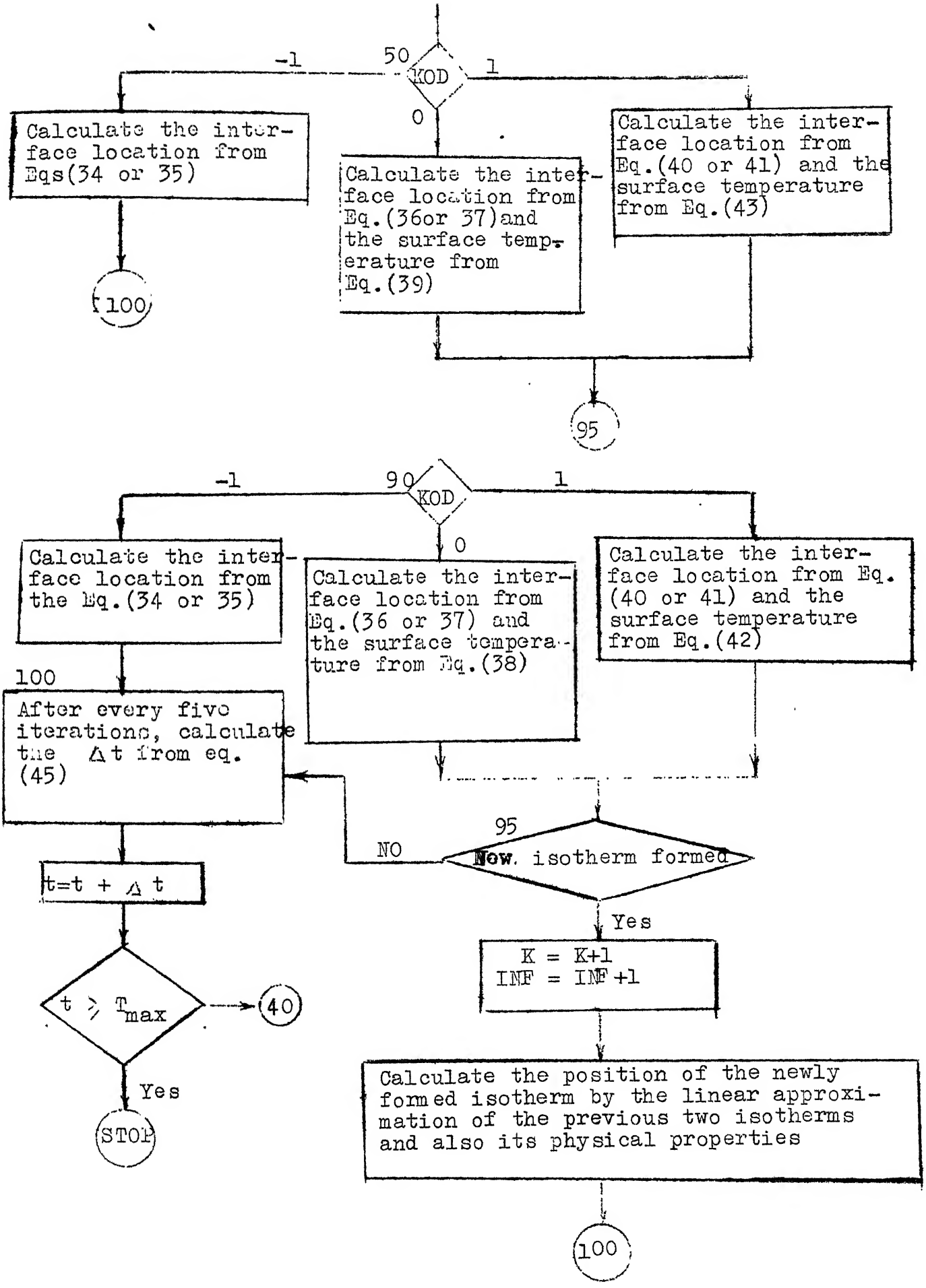
(d) Temperature dependent property (VIP)

= 1 Constant property
= 2 Variable property

(e) Inside/Outside Solidification (INOU)

= -1 Outside freezing in cylindrical/spherical geometry
= 1 Inside freezing in cylindrical/spherical geometry


START
10
INPUT DATA:
Initialise: Isotherms T(i), Position of the isotherms X(i,j) at time t; Maximum time (T_{max}); No. of isotherms (K); Interface isotherm(INT); Thermophysical properties (TKH(i), ALPSO, ALPLO, TKSO, TKLO, RHO, ALTEN, SPHS, SPHL etc.)
Codes for: Geometry type; Boundary conditions; Initial state of the liquid, Temperature dependent property, Direction of solidification
20
NIS
1
2
K=INT
30
VIP
1
2
Read RALP(i) for const.properties
Read RALP(i) for variable properties
40
Calculate the position of the isotherms, excluding the interface one, from the main governing Eq.(26)
45
N
0
2
1
90
50


50
KOD
-1
0
1
Calculate the interface location from Eqs(34 or 35)
Calculate the interface location from Eq.(36or 37)and the surface temperature from Eq.(39)
Calculate the interface location from Eq.(40 or 41) and the surface temperature from Eq.(43)
100
95
90
KOD
-1
0
1
Calculate the interface location from the Eq.(34 or 35)
Calculate the interface location from Eq.(36 or 37) and the surface temperature from Eq.(38)
Calculate the interface location from Eq.(40 or 41) and the surface temperature from Eq.(42)
100
After every five iterations, calculate the Δt from eq. (45)
95
NO
New isotherm formed
Yes
t=t + Δ t
t ≥ Tmax
40
Yes
STOP
K = K+1
INF = INF +1
Calculate the position of the newly formed isotherm by the linear approximation of the previous two isotherms and also its physical properties
100

CHAPTER 5

RESULTS AND DISCUSSION

Computations following the modified IMM with suitably chosen $\Delta\tau$ from Eq.(45) were performed for the solidification of water initially at $0^{\circ}C$ [saturated case] and at $20^{\circ}C$ [unsaturated case] on DEC 1090 computer. The boundary conditions chosen arbitrarily, are the followings:

(1) $\theta_w = -30^{\circ}C$ for B.C. of the 1st kind.

(2) $q_c\big]_{x=o} = 0.1$ cals/sec cm^2 for B.C. of the 2nd kind

(3) $h = 100$ Btu/hr.$ft^2{}^{\circ}F$ for B.C. of the 3rd kind

$= 4.18598 \times 10^{-3}$ cals/sec.cm^2 $^{\circ}C$

The physical properties of water and ice used in the study have been reported in the Appendix I. Results were obtained in the form of $X(i,j)$ as a function of time. They have been shown graphically for certain cases and compared with the available literature values. The legend for each of the cases has been labelled in the figure itself.

5.1 Results of the IMM for Solidification of Saturated Liquid Under Various Conditions:

Figs. (1 to 3) compare the IMM with the analytical solutions [4] showing the interface location and the temperature profiles for the Cartesion solidifying systems subjected to the boundary conditions of the 1st, 2nd and 3rd kind respectively.

It is found that for the B.C. of the 1st kind, the isotherms are closely spaced at small times and the spatial distance between any two isotherms increases with the passage of time. For the B.C. of the 2nd kind (Fig.2), the isotherms are more or less equally spaced throughout the time of solidification, since constant amount of heat is drawn all along the process from the surface; while for the B.C. of the 3rd kind (Fig.3) the spatial distance between any two consecutive isotherms increases slowly with time. For a given flux (Fig.2) and convection (Fig.3) at the boundary, the surface temperature decreases with time which causes the inclusion of the new isotherms at the boundary which afterwards keep on migrating through the medium.

Fig. 4 represents the comparison between the results of the IMM for equal and unequal temperature interval in $(T-\tau)$ grid. Here the temperature intervals are spaced at $0^{\circ}C$, $-5^{\circ}C$, $-15^{\circ}C$, $-25^{\circ}C$ and $-30^{\circ}C$ for the numerical calculation done by the IMM. The response is found to be good.

Fig. 5 depicts the interface location and the temperature profiles both for constant and the variable properties. In the constant property case, the properties are evaluated at the interface temperature, In the variable property case the initialisations of the IMM have been done from the modified error function solution [9]. The response follows the usual trend of the graph. Since the thermal conductivity of ice

increases with decreasing temperature [11] which facilitates the heat transfer through the body, both interface and other isotherms mi rate at a slightly faster rate than in the constant property case.

Fig.6 shows the comparison of the IMM with other approximate solutions [8] and [6] for depth of outward solidification through cylindrical and spherical bodies respectively. The results agree well. Here solidification is faster in case of the cylinder than in the case of the sphere. This is so because the increment of surface area resulting from solidification is more rapid in case of the cylinder than the sphere. This process facilitates the higher heat transfer and thereby higher migration rate of the interface in case of the cylinder.

For the inward solidification as shown in Fig.7, the effect of solidification on the surface area acts in the reverse way, wherein the sphere freezes faster than the cylinder. Here the complete solidification has been shown. This has been achieved by the extrapolation of the partial solidification calculated by the IMM upto the neighbourhood of the centre.

5.2 Results of the IMM for Solidification of Unsaturated Liquid Under Various Conditions:

In Fig.8 the results of the IMM have been compared with the Neumann's solution [4]. Here temperature profiles

have been calculated both in the solid and the liquid regions. The location of the last isotherm corresponding to $20^{o}C$ in the liquid region is calculated by the extrapolation technique, since no definite relation or boundary condition can be assigned to that point. Ideally, the temperature in the infinite medium asymptotically approaches its initial value T_s as 'X' becomes arbitrarily large. However, the concept of 'penetration distance' is used to locate the last isotherm in the liquid medium. For this purpose the following artifice is suggested. A parabola is fitted through X(i,j) of $10^{o}C$ isotherm and X(i,j) of $15^{o}C$ isotherm with $dT/dX = 0$ at $T=T_s$ ie at $20^{o}C$ isotherm. The distance at the point of **tangency** is taken as the penetration distance. Its value is given by

$$X(i,j) = \frac{X(i-1,j) - \sqrt{(T(i-1)-T(i))/(T(i-1)-T(i-2))}\cdot X(i-2,j)}{1 - \sqrt{(T(i-1)-T(i))/(T(i-1)-T(i-2))}}$$

Since the concept of the 'penetration distance' is not so well defined, the results of the IMM deviates from the analytical solutions [4] within 5 per cent for distant isotherms in the liquid region. However, in the solid zone the values are in good agreement with the Neumann's solution [4].

In Fig.(9), the results of the IMM for constant and variable properties with boundary condition of the 2nd kind have been plotted. Temperature fields are drawn both in the solid and in the liquid zone. The nature of the plots is

same as that of Fig.(2). In the unsaturated case, the interface and other isotherms migrate through the medium at a slower rate incomparison to the saturated case. The IMM Eq.(26) has been initialised from Boley's solution [15] for small time t=1 min. Since Boley's solution is based on finite geometry with one side insulated, if cannot be used to compare the results of the IMM for higher time.

The temperature profiles and the interface location for temperature dependent property and unequal temperature interval in a planer solidifying system have been shown in the Fig.(10). Comparison has also been made with equal temperature interval case. The results, thus obtained, are reasonably closed to each other.

Fig. (11) depicts the results of the IMM computed by the equal and the unequal temperature grids in the divided difference form. In unequal temperature interval case, the isotherms are randomly chosen at $-20^{o}C$, $-15^{o}C$, $-10^{o}C$, $0^{o}C$, $-1^{o}C$, $-3^{o}C$, $-5^{o}C$, $-8^{o}C$ etc. Here the system chosen is cylindrical body exposed to the boundary condition of the 3rd kind. The nature of the graph is satisfactory and the results in both the cases are reasonably closed to each other.

Fig.(12) shows the effect of property variation with temperature occurring in the spherical geometry. The temperature profiles in the solid and liquid zones and the position have been compared with the constant property case with the

properties evaluated at the interface temperature. The gradual increase of the thermal conductivity in the variable property case along the direction of heat flow facilitates the heat transfer and consequently the isotherms move at somewhat faster rate.

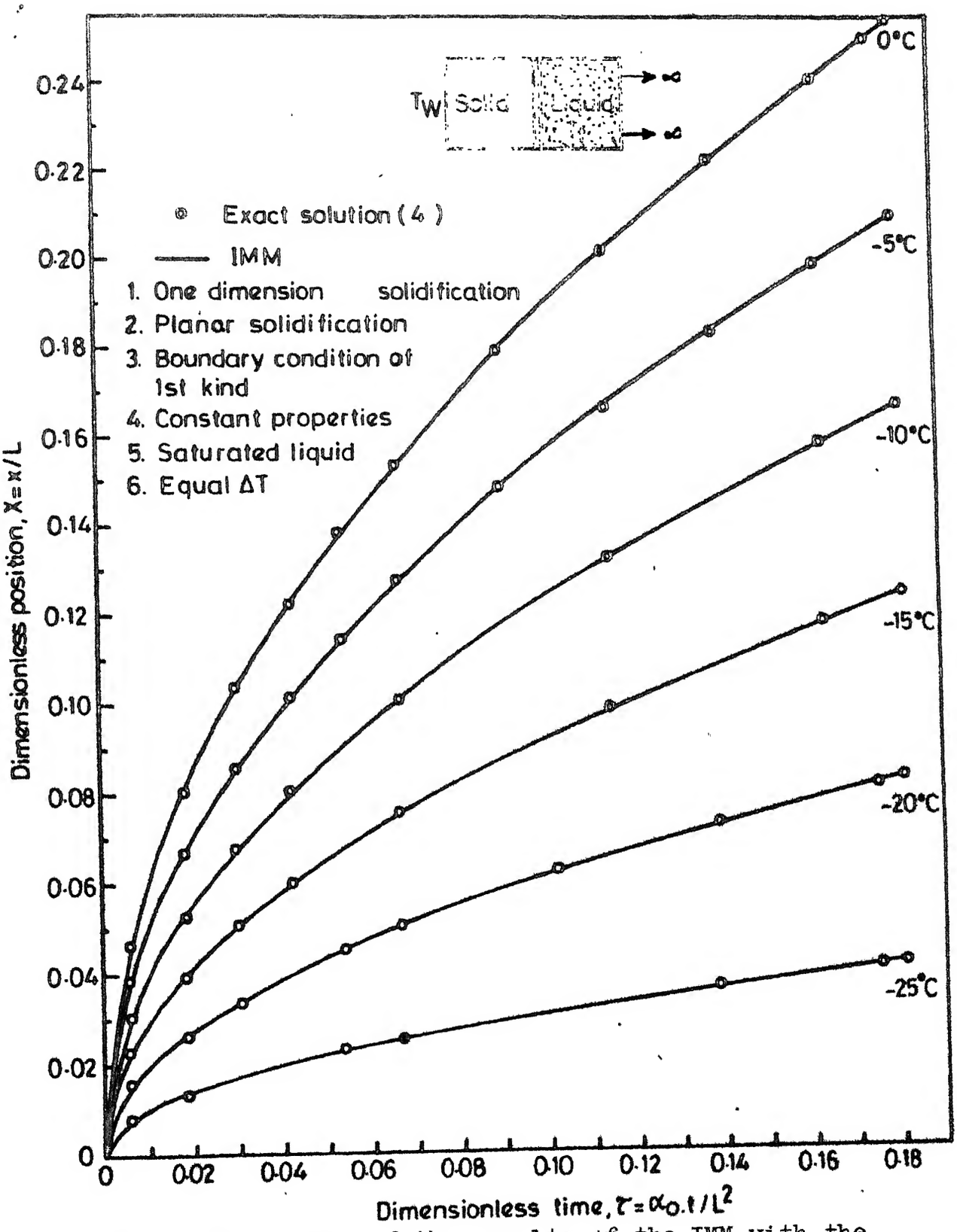


Fig.1: Comparison of the results of the IMM with the analytical solutions [4] for boundary condition of the 1st kind

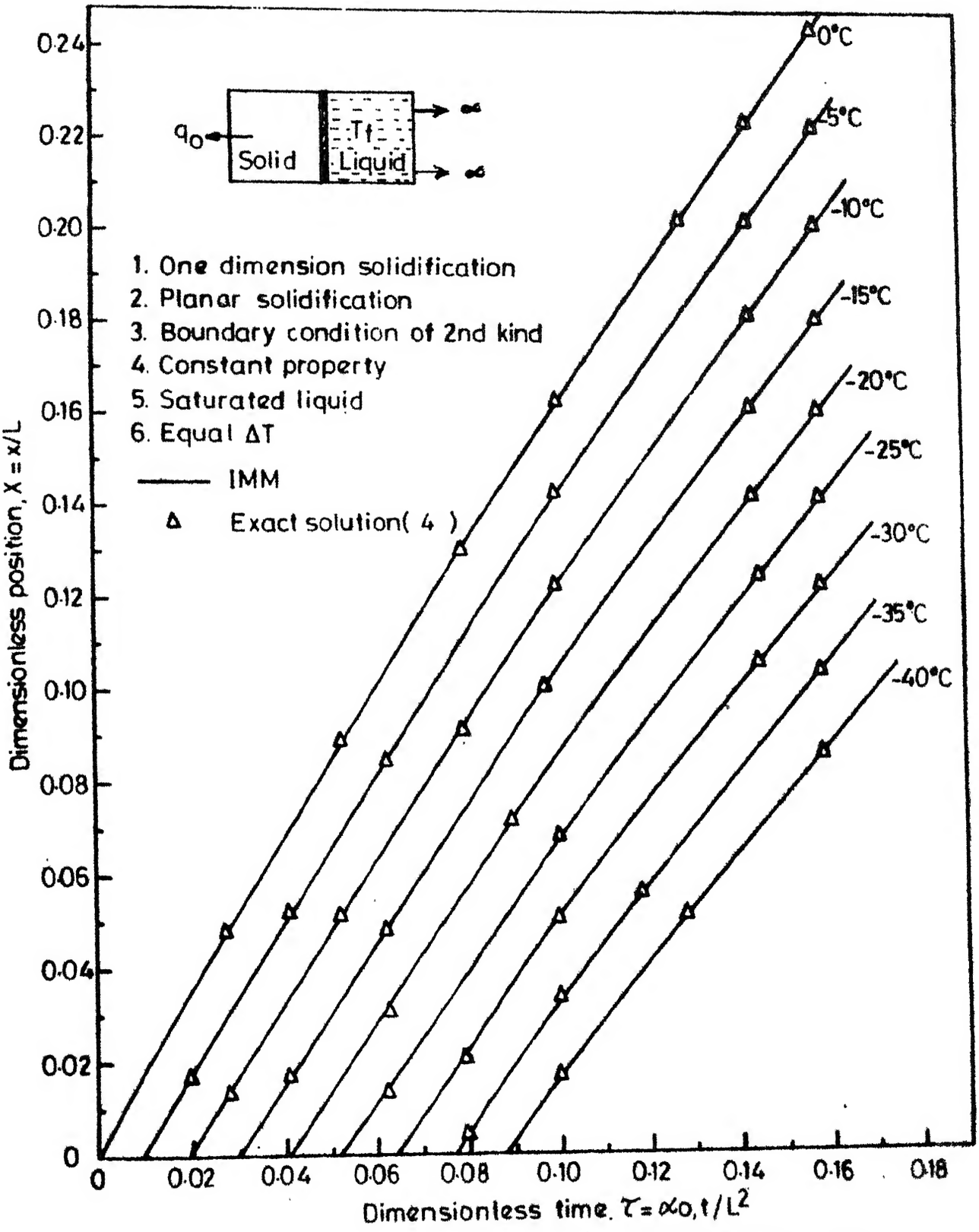


Fig.2: Comparison of the results of the IMM with the analytical solutions [4] for boundary cndition of the 2nd kind

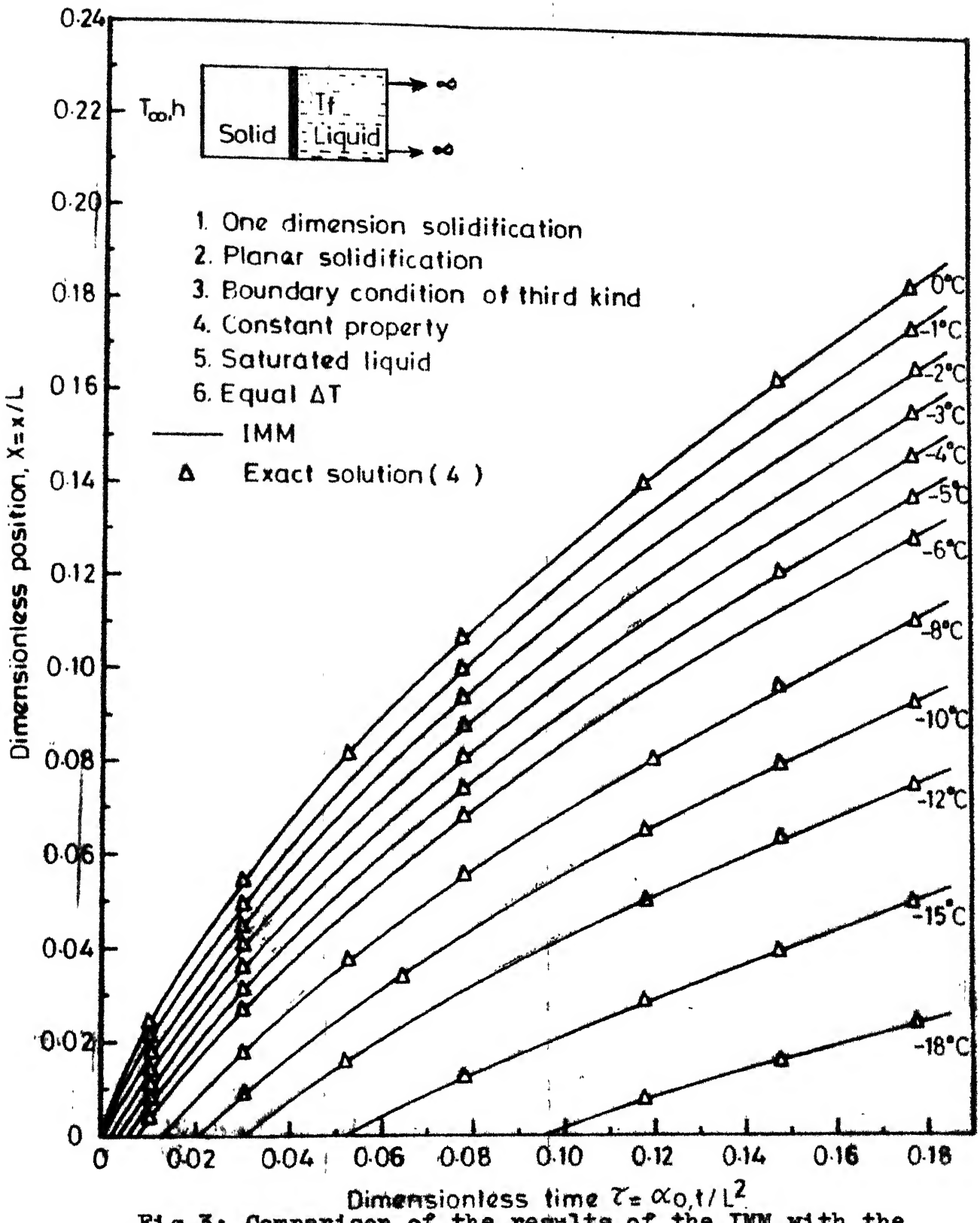


Fig.3: Comparison of the results of the IMM with the analytical solutions [4] for boundary condition of the 3rd kind

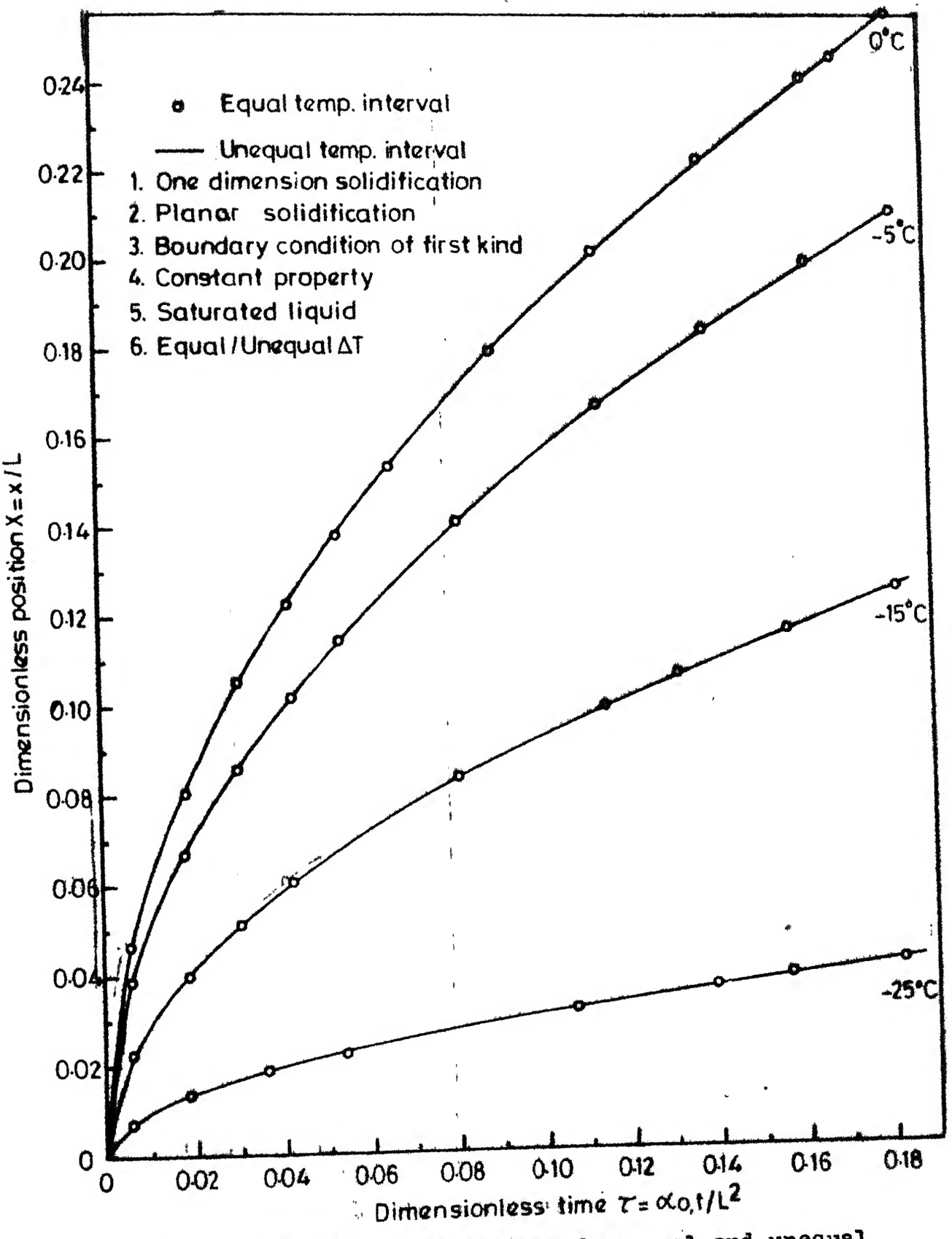


Fig.4: The results of the IMM for equal and unequal temperature intervals taken in the (τ-T) grid

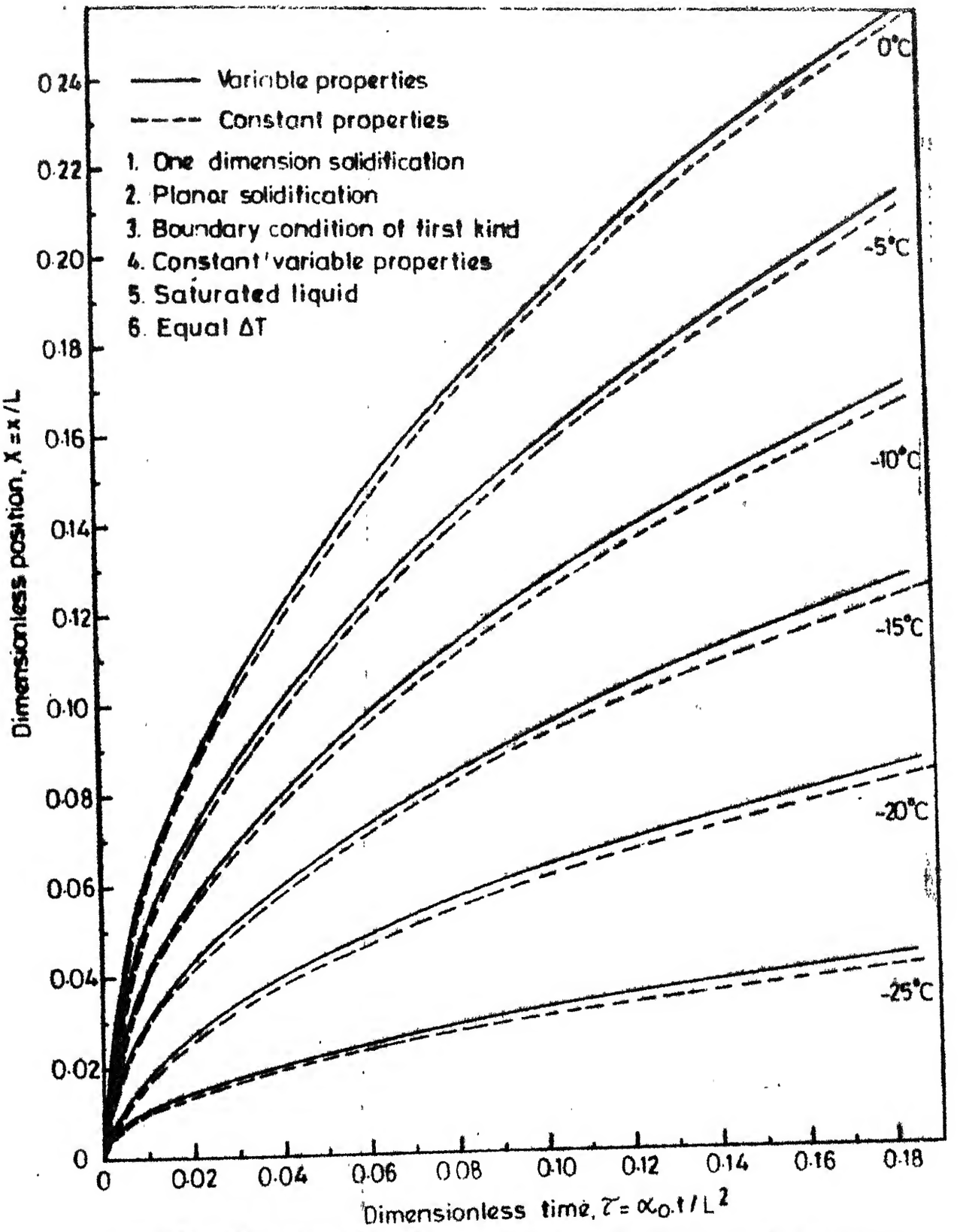


Fig.5: The results of the IMM for constant and variable property cases

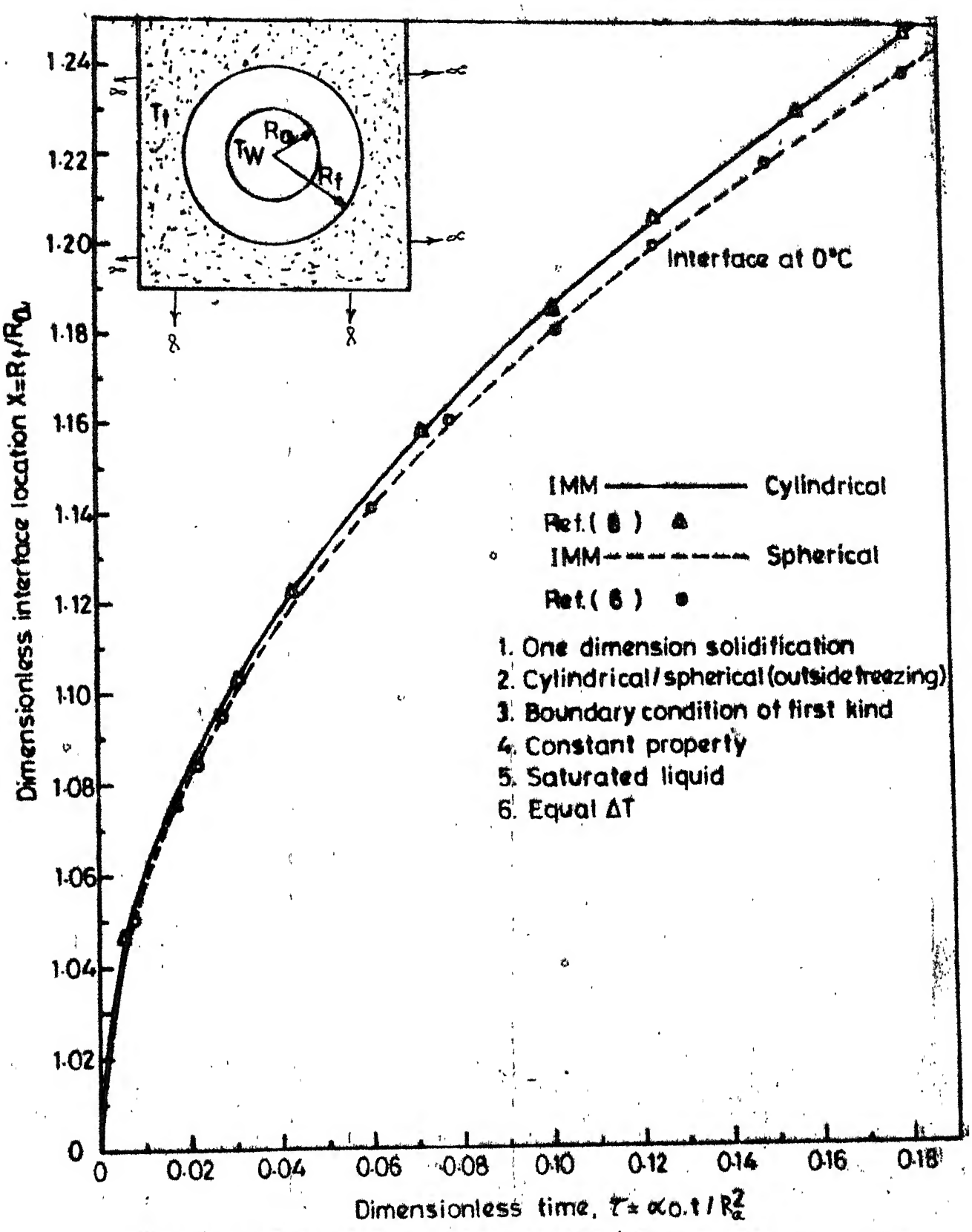


Fig.6: Comparison of the results of the IMM with other approximate solutions [8] and [6] for the depth of outward solidification through the cylindrical and spherical bodies respectively

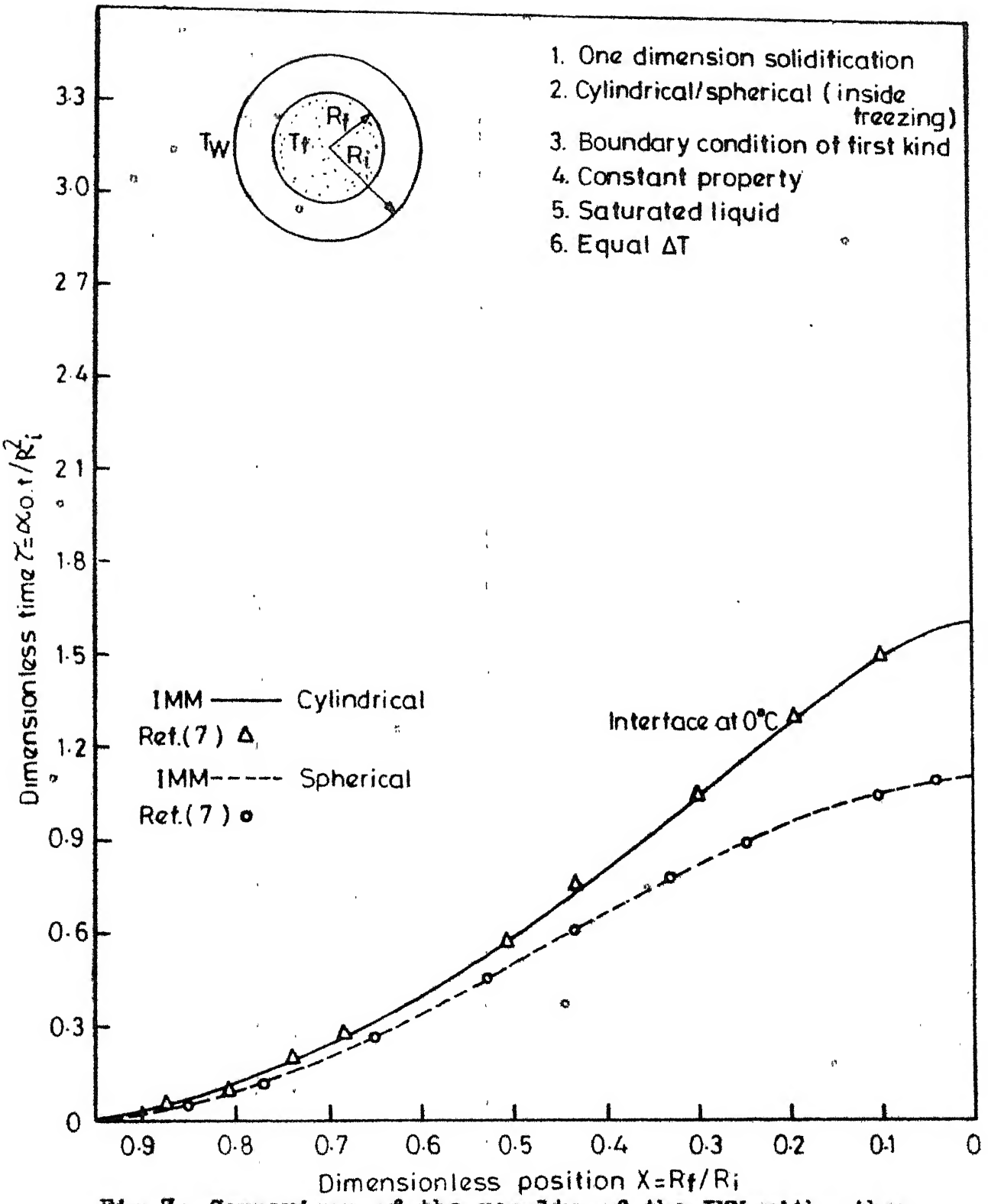


Fig.7: Comparison of the results of the IMM with other approximate solutions [7] for the depth of inward solidification through the cylindrical/spherical bodies

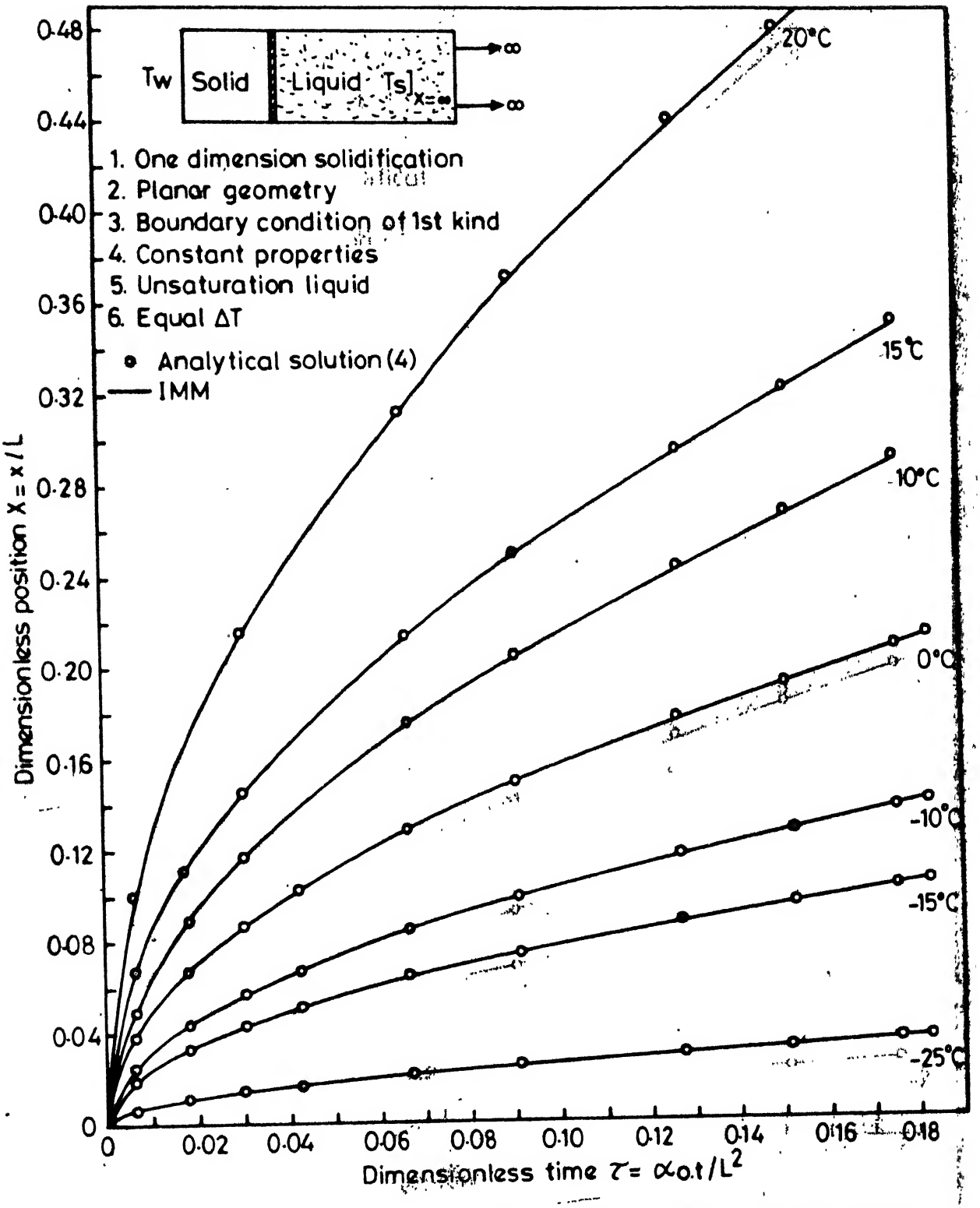


Fig. 8 - Comparison of the results of the IMM with Neumann's solution [4] for B.C. of the 1st kind.

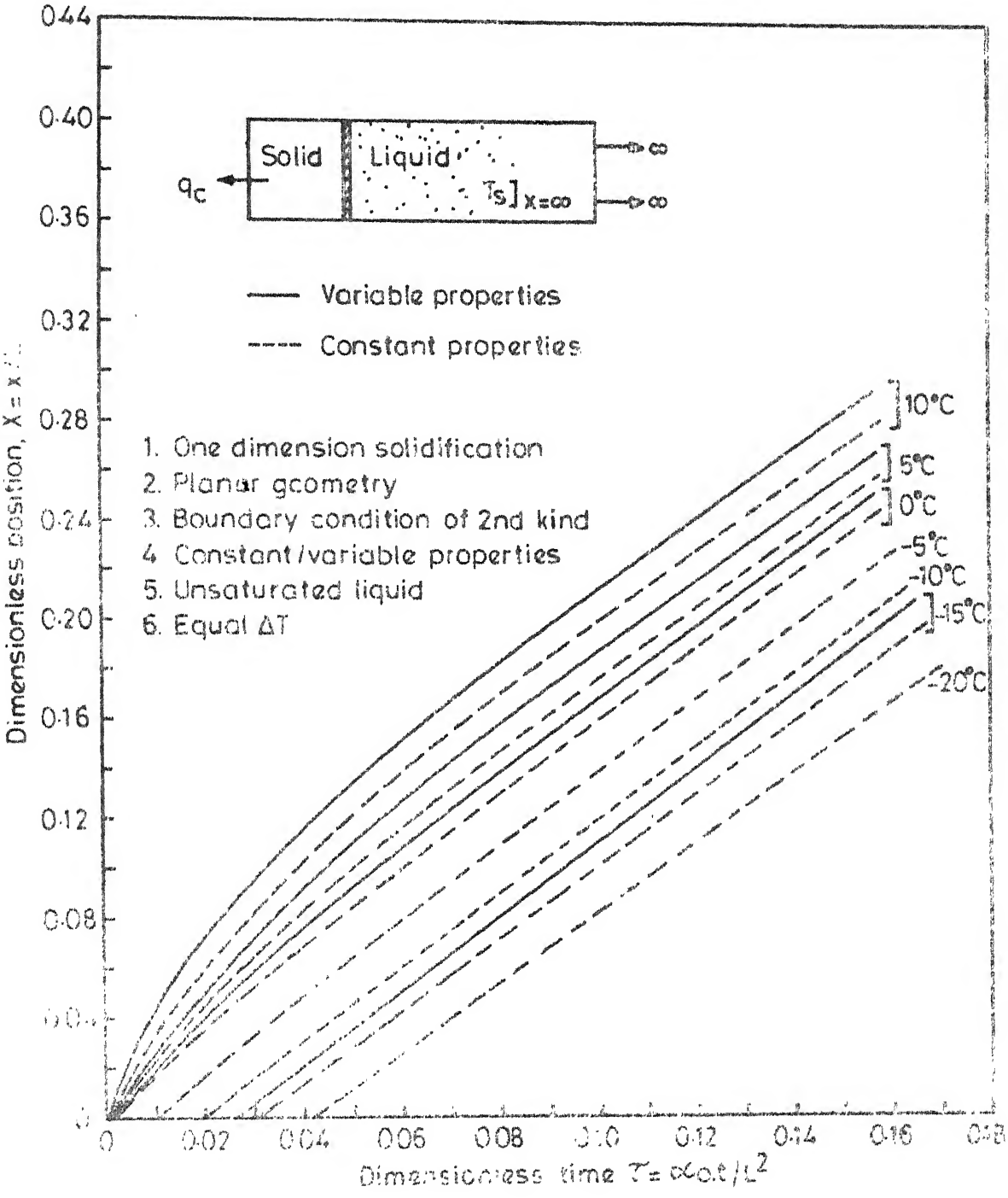


Fig 9 -The results of the IMM for constant and variable property cases with B.C. of the 2nd kind

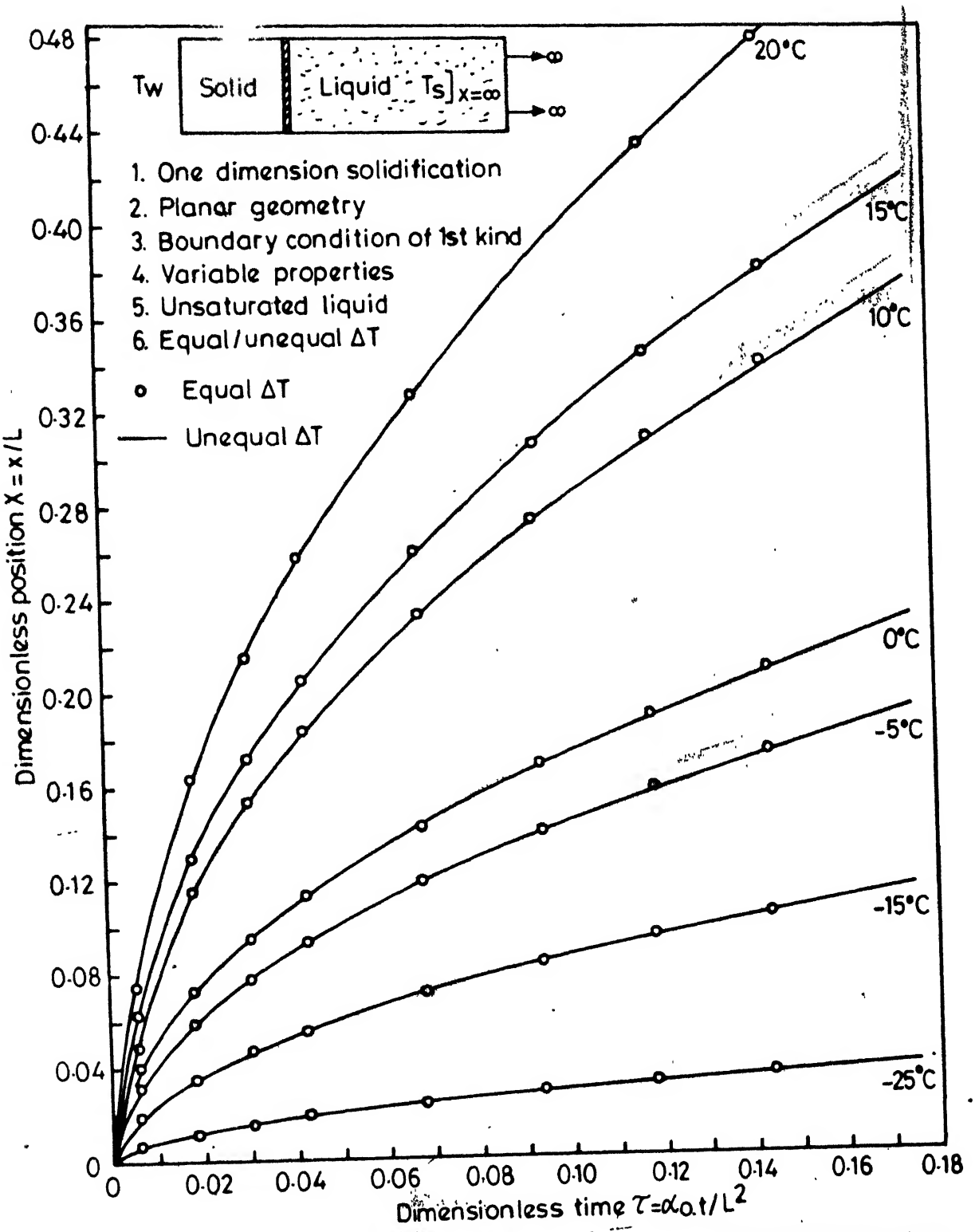


Fig. 10 -The results of the IMM for equal and unequal temperature interval in (τ-T) grid with temperature dependent properties.

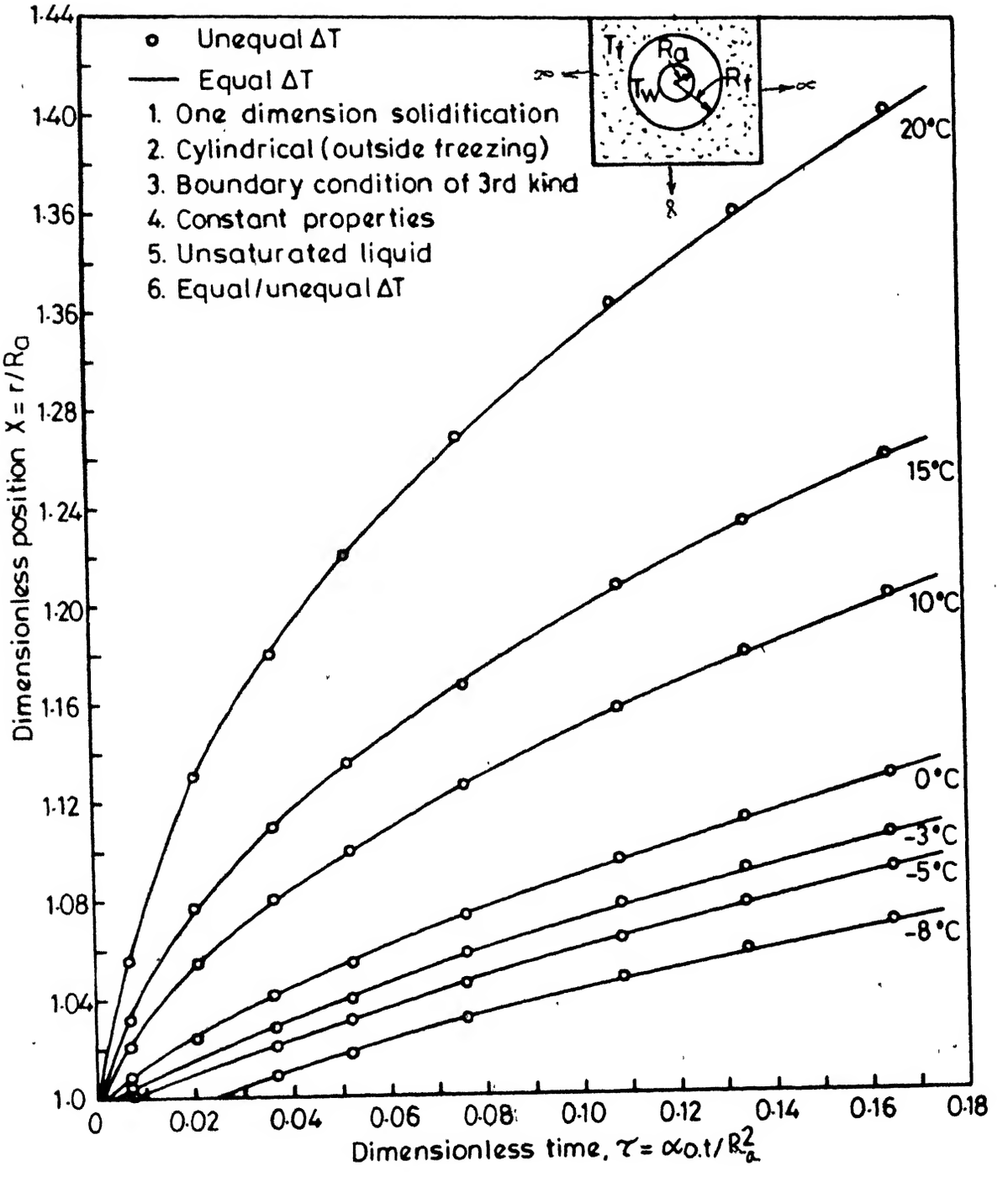


Fig. 11 - The results of the IMM for equal and unequal temperature interval in (τ-T) grid for B.C. of the 3rd kind.

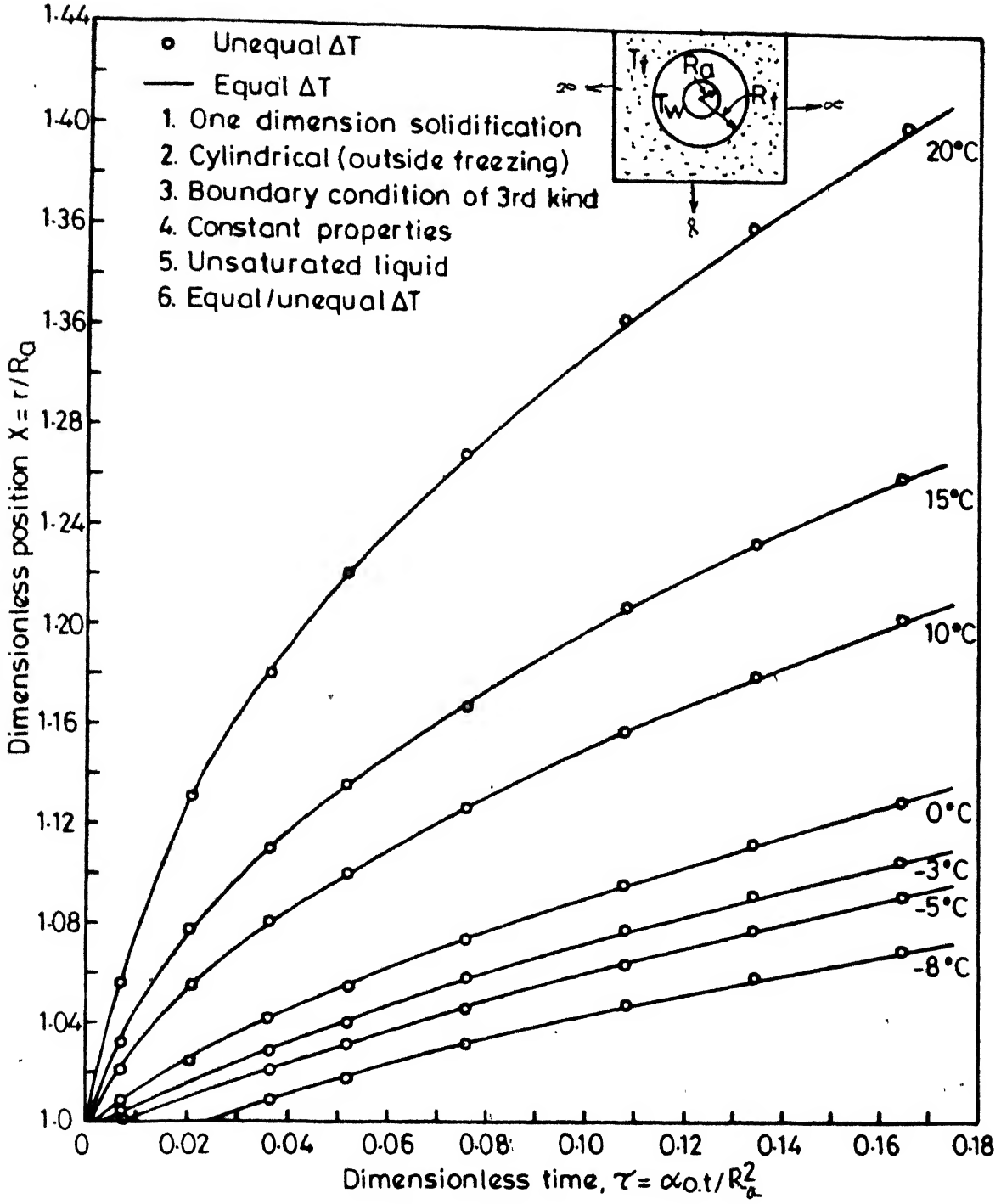


Fig. 11 - The results of the IMM for equal and unequal temperature interval in (τ-T) grid for B.C. of the 3rd kind.

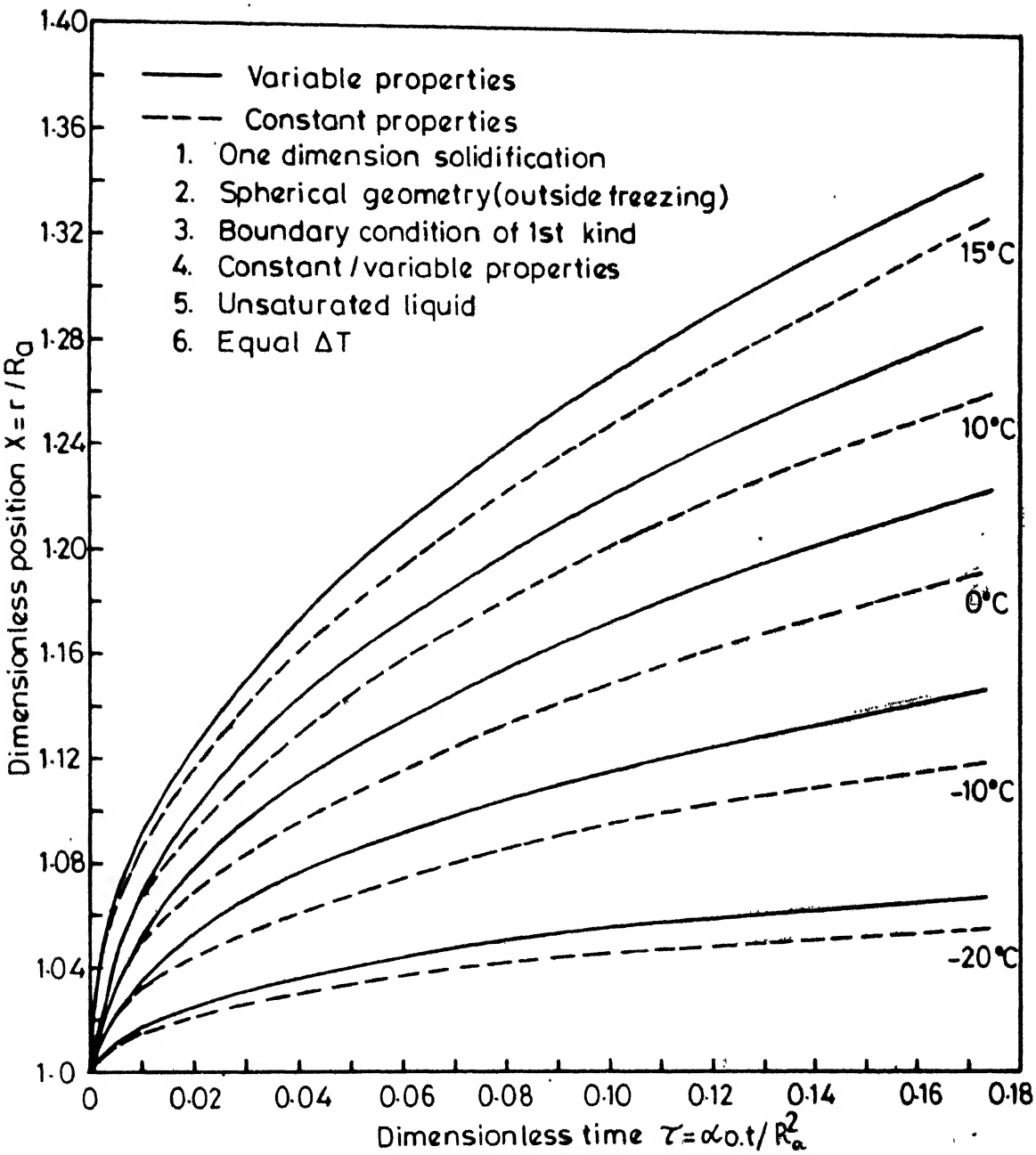


Fig. 12 -The results of the IMM for constant and variable property cases in spherical geometry.

CHAPTER 6

CONCLUSION

The above results in most of the cases compare with the literature values within 2 per cent. The deviation is slightly more (within 5 per cent) in the liquid region when the unsaturated liquid solidifies. To improve upon this one should look for better extrapolation techniques for locating the initial temperature isotherm. Convection in the liquid is ignored. However, the major effects of variation of the thermal conductivities and heat capacities have been studied. Hence, the analysis presented here permits a realistic evaluation of the interface location and temperature fields for unidimension solidification incorporating both the equal and unequal temperature interval in the time-temperature grids.

Though it is not a very major advance, it does increase the utility of the IMM quite a bit. Concentration dependent diffusivity problems in mass transfer operations can be solved similarly. Future work can be directed towards extension of the method to two and three dimension and the development of implicit method of solution of the equations. This modified IMM will be one important numerical tool to facilitate the multiphase solidification problems involved in the casting of steel and other alloys.

Based upon the discussion during the thesis defence, the following has been added.

(a) Radiation Boundary Condition:

The boundary condition for radiation at the surface X=0 and τ 0, can be expressed in the dimensionless form as

$$K \frac{\partial T}{\partial X} = h_r \cdot L \cdot T_w \qquad (A)$$

where h_r is radiation heat transfer coefficient

$$= \frac{\delta F_A F_e (T_w^4)}{T_w}$$

δ is Stefan-Boltzman constant, cals/sec $cm^2 (^oC)^4$

F_A is view factor, here $F_A = 1$

F_e is emissivity factor $= \dfrac{1}{\frac{1}{\varepsilon_1} + \frac{1}{\varepsilon_2} - 1}$

Substituting all these in Eq.(A), we have

$$\partial T / \partial X = \frac{\delta F_e L T_w^4}{K}$$

Taking divided difference form, we have

$$T_w = T(2) - \frac{\delta F_e L}{K} X (2, J+1) T_w^4$$

or

$$\frac{\delta F_e L X(2,J+1)}{K} \cdot T_w^4 + T_w - T(2) = 0 \qquad (B)$$

T_w can be calculated from the expression (B) by Regular Falsi Method. Once the surface temperature is known, the remaining procedure is same as that of other boundary conditions already discussed.

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APPENDIX I

The Physical Properties of Ice and Water and Their Temperature Dependences

(A) The required thermophysical properties of ice and water at $0^{\circ}C$ [11] are listed below:

Properties	Ice	Water	Units
Density(ρ)	0.92	0.99986	gms/cm^3
Specific heat (C)	0.492	1.0092	cals/gm $^{\circ}C$
Thermal conductivity (K)	49.9205×10^{-4}	13.25×10^{-4}	cals/sec cm $^{\circ}C$
Thermal diffusivity(α)	0.0114	1.321×10^{-3}	cm^2/sec

The latent heat of solidification of water is

$$\lambda = 79.78 \text{ cals/gm.}$$

(B) The variations of the specific heat of ice with temperature [11] are as follows:

Temperature, $^{\circ}C$	Specific heat of ice, cals/gm $^{\circ}C$
0	0.492
-20	0.4633
-40	0.4346

For small temperature range, it has been evaluated from the relation

$$C = a + bt + ct^2 \quad \text{where t is in } ^{\circ}C$$

$$a = 0.492; \quad b = -3.5875 \times 10^{-5} \quad \text{and}$$

$$c = 1.793 \times 10^{-5}$$

(c) The variations of the specific heat of water with temperature [11] are as follows:

Temperature, ^{o}C	Specific heat, cals/gm ^{o}C
0	1.0092
5	1.0051
10	1.0021
15	1.0001
20	0.9983

(d) The thermal conductivity of ice varies with temperatures [11] according to the relation

$$K_t = K_o [1 - 17 \times 10^{-4} t] \quad -170^{o}C < t < 0^{o}C$$

where t is in ^{o}C

and $K_o = 49.9205 \times 10^{-4}$ cals/sec cm.^{o}C

(e) The variation of the thermal conductivity of water with temperatures has been reported in literature [11], according to the relation

$$K_t = K_{20} [1+0.00281 (t-20)], \quad 0^{o}C < t < 80^{o}C$$

where t is in ^{o}C

and $K_{20} = 1.420 \times 10^{-3}$ cals/sec. cm ^{o}C.

No definite relation or discreate values for thermal diffusivity with temperature have been found in the literatures. So it has been calculated from the relation $\alpha = K/\rho C$, where K and C are evaluated at the required temperature from the above correlations.

```
C
C
C
C       COMPUTER PROGRAMMING FOR
C     ******************************************************************
C     ISOTHERM ,MIGRATION ,METHOD ,  (I,M,M)
C     ******************************************************************
C
C     ONE DIMENSIONAL PHASE CHANGE PROBLEM(SOLIDIFICATION OF WATER)IN
C     CARTESIAN,CYLINDRICAL AND SPHERICAL SYSTEM, CONSTANT/ VARIABLE
C     PROPERTIES,EQUAL/UNEQAL TEMPARATURE INTERVALS,LIQUID IS AT
C     SATURATED/UNSATURATED STATE,THE SYSTEM IS SUBJECTED TO THE
C     BOUNDARY CONDITIONS OF THE 1ST/2ND/3RD KIND,THE VALUE REQUIRED
C     TO START THE ALGORITHIM IS FED BY HAND COMPUTATION FROM NEUMANS
C     SOLUTIONS
C
C     ******************************************************************
C
C     DEFINATION OF DIFFERENT PARAMETERS USED IN THE PROGRAM
C
C     ******************************************************************
C       I       = TEMPERATURE GRID INDEX
C       J       = TIME GRID INDEX
C       N       = A FACTOR TO IDENTIFY THE COORDINATE SYSTEM,N=0 PLANER,
C                 N=1 CYLINDRICAL AND N=2 SPHERICAL CORDINATE
C       K       = TOTAL NUMBER OF ISOTHERM IN THE SOLID AND LIQUID
C                 ZONE INCLUCING THE INTERFACE ONE
C       NIS     = A FACTOR TO REPRESENT THE INITIAL STATE OF THE
C                 LIQUID;NIS=1,SATURATED ;NIS=2,UNSATURATED LIQUID
C       VIP     = A FACTOR TO INCORPORATE PROPERTY VARIATION WITH
C                 TEMP. VIP=1,CONST.PROP.;VIP=2,VARIABLE PORP.
C       INOU    = A FACTOR TO REPRESENT INWARD/OUTWARD SOLIDIFICATION
C                 FOR CYLINDRICAL/SPHERICAL GEOMETRIES;INOU=1,INSIDE
C                 OR PLANER SOLIDIFIC.;INOU=-1,OUTSIDE SOLIDIFIC.
C       KOD     = A FACTOR TO REPRESENT DIFFERENT BOUNDARY CONDITIONS
C                 KOD=-1,1ST.KIND;KOD=0,2ND.KIND;KOD=1,3RD.KIND
C       INF     = A COUNTER TO SPECIFY THE INTERFACE ISOTHERM
C       ALPSO   = THERMAL DIFFUSIVITY OF THE SOLID AT THE
C                 INTERFACE TEMPARATURE
C       ALPLO   = THERMAL DIFFUSIVITY OF THE LIQUID AT THE
C                 INTERFACE TEMPARATURE
C       ALP(I)  = THERMAL DIFFUSIVITY OF THE ITH ISOTHERM
C       RALP(I)= ALP(I)/ALPSO    OR   TKH(I)/TKSO
C       TKSO    = THERMAL CONDUCTIVITY OF THE SOLID AT THE
C                 INTERFACE TEMPERATURE
C       TKLO    = THERMAL CONDUCTIVITY OF THE LIQUID AT THE
C                 INTERFACE TEMPERATURE
C       TKH(I)  = THERMAL CONDUCTIVITY OF THE ITH ISOTHERM
C       RHO     = DENSITY OF SOLID OR LIQUID (ASSUMING CONSTANT)
C       X(I,J)  = DIMENSIONLESS POSITION OF THE ITH ISOTHERM AT JTH TIME
C       T(I)    = DIMENSIONLESS TEMPARATURE OF THE ITH ISOTHERM
C                 DEFINED IN THE TEXT
C       SPHS    = SPECIFIC HEAT OF THE SOLID
C       SPHL    = SPECIFIC HEAT OF THE LIQUID
C       AL      = SUTABLY CHOSEN A PARAMETER IN DIMENSION OF LENGTH
C       TAUMAX  = MAXIMUM TIME UP TO WHICH THE RESULT IS REQUIRED
C       STIME   = THE SMALL STARTING TIME AT WHICH THE ALGORITHM
C                 HAS BEEN INITIALISED
C       DELTAU  = DIMENSIONLESS TIME INCREMENT=(ALPSO*TIME)/AL**2
C       CAT     = THE COEFFICIENT OF CALCULATED DELTAU TO INCORPORATE
C                 STABILITY CRITERION FOR NONLINEAR EQUATION
C       H       = HEAT TRANSFER COEFFICIENT OF THE SURROUNDINGS
C       FLUX    = CONSTANT HEAT FLUX DRAWN FROM THE SURFACE
C     ******************************************************************
```

```
0100    C
0200    CC
0300    C
0400    C
0500            DIMENSION T(45),X(45,1000),TKH(45),S(45),Y(45,1000),TKG(45)
0600            5,RALP(25),GALP(25)
0700            READ(1,5)K,NIS,INF,N,INOU,KOD
0800    5       FORMAT(6I3)
0900            TYPE151
1000    151     FORMAT(//,10X,'VALUE OF DIFFERENT FACTORS USED IN THE PROGRAM')
1100            TYPE152
1200    152     FORMAT(10X,'-------------------------------------------------')
1300            TYPE161,K,NIS,INF,N,INOU,KOD
1400    161     FORMAT(//,2X,'K=',I3,5X,'NIS=',I3,5X,'INF=',I3,5X,'N=',I3,
1500            25X,'INOU='I3,5X,'KOD='I3)
1600            READ(1,10)ALPSO,ALPLO,RHO,DELTAU,SPHS,SPHL,ALATEN,TKSO,
1700            5TKLO,VIP,CAT
1800    10      FORMAT(6F9.6)
1900            TYPE111
2000    111     FORMAT(//,10X,'PHYSICAL PROPERTIES OF WATER AND ICE AT 0C')
2100            TYPE121
2200    121     FORMAT(10X,'-------------------------------------------------')
2300            TYPE131,ALPSO,ALPLO,RHO,DELTAU,SPHS,SPHL
2400    131     FORMAT(//,2X,'ALPSO=',F9.6,2X,'ALPLO=',F9.6,2X,'RHO=',F9.6,2X,
2500            5'DELTAU=',F9.6,2X,'SPHS=',F9.6,2X,'SPHL=',F9.6)
2600            TYPE141,ALATEN,TKSO,TKLO,VIP,CAT
2700    141     FORMAT(//,2X,'ALATEN=',F9.6,2X,'TKSO=',F9.6,2X,'TKLO=',
2800            5F9.6,2X,'VIP=',F9.6,2X,F5.2)
2900            TIMAX=3600.0;STIME=120.0;AL=15.0
3000            TAUMAX=(ALPSO*TIMAX)/(AL**2);STAU=(ALPSO*STIME)/(AL**2)
3100            IF(NIS.EQ.1)K=INF
3200            READ(1,20)(T(I),I=1,K)
3300    20      FORMAT(7F7.5)
3400            READ(1,30)(X(I,1),I=1,K)
3500    30      FORMAT(6F9.7)
3600            READ(1,40)(TKH(I),I=1,K)
3700            IF(VIP.EQ.1)GOTO35
3800            READ(1,10)(RALP(I),I=1,K)
3900    40      FORMAT(6F10.8)
4000    35      H=4.18595E-03;TINF=0.0;FLUX=0.1
4100            IF(KOD.EQ.1)DTEM=0.03333
4200            IF(KOD.EQ.0)DTEM=0.00333
4300            IF(VIP.EQ.1.0)RALP(1)=1.0
4400            TYPE42,(T(I),I=1,K)
4500    42      FORMAT(//,2X,'SPECIFIED ISOTHERMS ARE'/1X,11(2X,F7.5))
4600            TYPE59
4700    59      FORMAT(1X,'-------------------------------------------------')
4800            TYPE43,(X(I,1),I=1,K)
4900    43      FORMAT(//,2X,'INITIAL POSITION OF THE ISOTHERMS'/1X,11(1X,F9.7))
5000            TYPE59
5100            IF(N.EQ.2)GOTO100
5200            IF(N.EQ.1)GOTO200
5300            TYPE11
5400    11      FORMAT(///,15X,'PLANNER  SOLUTIONS'///)
5500            GOTO300
5600    100     TYPE22
5700    22      FORMAT(///,15X,'SPHERICAL  SOLUTIONS'///)
5800            GOTO300
5900    200     TYPE33
6000    33      FORMAT(///,15X,'CYLINDRICAL SOLUTIONS'///)
6100    300     J=1;JO=1;TKSO=0.499205E-02
6200            KOUNT=1
6300            TAU=STAU+DELTAU;TL=STAU;TAUIM=0.180;NAT=0
```

```
00100     C
00200     CCC
00300     CCCC
00400     CCCC
00500     CCCC        CALCULATION OF THE ISOTHERM POSITION IN THE FROZEN AND
00600     CCCC        ------------------------------------------------------------
00700     CCCC        UNFROZEN REGION
00800     CCCC        -------------------
00900     302         DO400I=2,K
01000     69          IF(I.EQ.K)GOTO900
01100                 IF(KOD.GE.0)GOTO79
01200                 X(1,J+1)=1.0
01300                 IF(N.EQ.0)X(1,J+1)=0.0
01400     79          IJ=J+1
01500                 XI=(X(I+1,J)-X(I-1,J))
01600                 XA=X(I+1,J)*(T(I)-T(I-1))
01700                 XB=X(I-1,J)*(T(I+1)-T(I))
01800                 TI=(T(I+1)-T(I-1))
01900                 TT=(T(I+1)-T(I))*(T(I)-T(I-1))
02000                 TTI=(2.0*TI)/(TT*(XI**2))
02100                 INF2=INF+1
02200                 IF(I.EQ.INF2)TKH(I-1)=TKLO
02300                 TKI=(TKH(I+1)-TKH(I-1))
02400                 IF(VIP.EQ.1)TKI=0.0
02500                 IF(VIP.EQ.1.)RALP(I)=1.0
02600                 IF(NIS.EQ.1)GOTO500
02700                 IF(I.EQ.INF)GOTO600
02800                 IF(I.GT.INF.AND.VIP.EQ.1)RALP(I)=0.1158771
02900     500         T1=RALP(I)*DELTAU*TTI
03000                 T2=T1*TI
03100                 T3=RALP(I)*DELTAU
03200                 X(I,J+1)=(T1*(XA+XB))+((1.-T2)*X(I,J))-((T3*N)/X(I,J))
03300                 5-((T3*TKI)/(TKH(I)*XI))
03400                 GOTO400
03500     600         SHS=(X(I,J)-X(I-1,J))/(T(I)-T(I-1))
03600                 SHL=(X(I+1,J)-X(I,J))/(T(I+1)-T(I))
03700                 IF(KOD)76,77,76
03800     C           CALCULATION OF THE INTERFACE POSITION FOR UNSATURATED CASE
03900     C           ------------------------------------------------------------
04000     76          X(I,J+1)=X(I,J)+(DELTAU)*((TKSO*30./SHS)+(TKLO*20./
04100                 5SHL))/(ALPSO*RHO*ALATEN)
04200                 GOTO400
04300     77          X(I,J+1)=X(I,J)+(DELTAU*FLUX*AL)*((1./SHS)-(TKLO/SHL*TKSO))/
04400                 5(ALPSO*RHO*ALATEN)
04500                 GOTO400
04600     900         IF(NIS.EQ.1)GOTO700
04700     C           CALCULATION OF THE POSITION OF THE FARTHEST ISOTHERM IN THE
04800     CC          UNFROZEN REGION BY PARABOLA FITTING METHOD
04900     C           ------------------------------------------------------------
05000                 TSK=SQRT((T(I-1)-T(I))/(T(I-2)-T(I)))
05100                 X(I,J+1)=(X(I-1,J+1)-TSK*X(I-2,J+1))/(1-TSK)
05200                 GOTO400
05300     700         SH2=(X(I,J)-X(I-1,J))/(T(I)-T(I-1))
05400     C           CALCULATION OF THE INTERFACE POSITION FOR SATURATED CASE
05500     C           ------------------------------------------------------------
05600                 IF(KOD)82,83,82
05700     82          X(I,J+1)=X(I,J)+(DELTAU*SPHS*30.0)/(SH2*ALATEN)
05800                 GOTO400
05900     83          X(I,J+1)=X(I,J)+(FLUX*DELTAU*AL)/(ALPSO*RHO*ALATEN*SH2)
06000     400         CONTINUE
06100                 IF(KOD)4000,14,13
06200     4000        IF(J.GE.7)GOTO710
06300     720         TYPE1000,J,TAU,DELTAU,(X(I,J+1),I=1,K)
06400     1000        FORMAT(/,2X,'J=',I7,2X,'TAU=',F9.7,2X,'DELTAU=',F10.8,/1X,11
06500                 5(1X,F9.7))
06600                 GOTO796
06700     710         IF(TAU.GE.TAUIM)GOTO720
06800                 IF((TAU-TL).GE.0.012)GOTO730;GOTO796
06900     730         TYPE1000,J,TAU,DELTAU,(X(I,J+1),I=1,K);TL=TAU
07000                 GOTO796
```

```
0100    C
0200    C
0300    C
0400    C
0500    C       AFTER EVERY ITERATION THE INCLUSION OF THE NEW ISOTHERM
0600    C       IS CHECKED FOR THE BOUNDARY CONDITIONS OF 2ND&3RD KIND
0700    C       ------------------------------------------------------------
0800    14      IF(N.GE.1)TWN=(T(2)+INOU*(1.-X(2,J+1)))/RALP(1)
0900            IF(N.EQ.0)TWN=(T(2)+INOU*(0.0-X(2,J+1)))/(TKH(1)/TKSO)
1000            GOTO86
1100    13      IF(N.GE.1)FACT=((1.-X(2,J+1))*H*AL)/TKH(1)
1200            IF(N.EQ.0)FACT=(X(2,J+1)*H*AL)/TKH(1)
1300            TWN=T(2)/(1.+INOU*FACT)
1400            IF(TWN.LE.TINF)GOTO202
1500    86      TDIF=T(1)-TWN
1600            IF(N.EQ.0)X(1,J+1)=X(2,J+1)*((T(1)-TWN)/(T(2)-TWN))
1700            IF(N.GE.1)X(1,J+1)=1.+(X(2,J+1)-1.)*((T(1)-TWN)/(T(2)-TWN))
1800            ODIF=(DTEM-TDIF);IF(ODIF)39,39,49
1900    49      IF(J.GE.2)GOTO796
2000            GOTO820
2100    39      DO41 II=1,K
2200    41      S(II)=T(II)
2300            DO51 II=1,K
2400    51      Y(II,J+1)=X(II,J+1)
2500            DO71II=1,K
2600            GALP(II)=RALP(II)
2700    71      TKG(II)=TKH(II)
2800            K=K+1
2900            INF=INF+1
3000    C       NEW ISOTHERM IS ADDED IN THE SYSTEM
3100    C       ------------------------------------------------------
3200            DO444I=2,K
3300            T(I)=S(I-1)
3400    444     CONTINUE
3500            T(1)=T(1)-DTEM
3600            DO555I=2,K
3700            X(I,J+1)=Y(I-1,J+1)
3800    555     CONTINUE
3900    C       LOCATION OF THE NEW ISOTHERM BY LINEAR APPROX.WITHIN
4000    C       ------------------------------------------------------------
4100    C       SMALL TEMPERATURE INTERVAL
4200    C       ------------------------------------------------------
4300            IF(N.EQ.0)X(1,J+1)=X(2,J+1)*((T(1)-TWN)/(T(2)-TWN))
4400            IF(N.GE.1)X(1,J+1)=1.+(X(2,J+1)-1.)*((T(1)-TWN)/(T(2)-TWN))
4500            DO666I=2,K
4600            RALP(I)=GALP(I-1)
4700    666     TKH(I)=TKG(I-1)
4800    C       CAL CULATION OF THE THERMAL CONDUCTIVITY AND THERMAL
4900    C       DIFFUSIVITY OF THE NEW ISOTHERM ACCORDING TO LINEAR
5000    C       APPROXIMATION AS REPORTED IN THE LITERATURE
5100    C       ------------------------------------------------------------
5200            IF(VIP.GT.1.0.AND.KOD.EQ.1)TKH(1)=TKSO*(1.-0.051*(T(1)-1.))
5300            IF(VIP.GT.1.0.AND.KOD.EQ.0)TKH(1)=TKSO*(1.-0.5108*T(1))
5400            IF(VIP.GT.1.)RALP(1)=RALP(2)+(RALP(K-5)-RALP(2))*(T(1)-T(2))/
5500            5(T(K-5)-T(2))
5600            IF(VIP.EQ.1.0)TKH(1)=TKSO
5700            IF(VIP.EQ.1.0)RALP(1)=1.0
5800            TYPE2000,KOUNT,J,TAU,DELTAU,TWN,(X(I,J),I=1,K-1)
5900    820     TYPE2000,KOUNT,IJ,TAU,DELTAU,TWN,(X(I,J+1),I=1,K)
6000    2000    FORMAT(2X,I5,2X,I7,2X,F12.6,2X,F10.8,2X,F9.5/1X,9(1X,E13.8))
6100    796     J=J+1;TAU=TAU+DELTAU
6200            IF(TAU.GE.TAUMAX)GOTO202
6300            IF(J.GE.998)GOTO204
6400            JJ=J-JO
6500            IF(JJ.GE.10)GOTO203
6600            GOTO302
```